Computational Study of Turbulent Partially-Premixed Flame with Inhomogeneous Inlets

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1 Introduction

Compositional inhomogeneity term is referred as wide range of mixture fractions in a fluid parcel, which includes both flammable and non-flammable fluid. It is often found in practical combustion devices like gas turbine engines [1], gasoline direct injection engines [2] and diesel engines [3]. An experimental setup to study the effects of compositional inhomogeneity at inlets in terms of flame stability has been developed by Meares et al. [4] and Barlow et al. [5]. Their experimental study shows increase in flame stability with compositional inhomogeneity due to existence of stratified-premixed combustion near jet exit plane. It is found that stratified-premixed combustion near jet exit plane causes additional heat release which augments the stabilizing effect of pilot.

Large eddy simulation (LES) is a promising tool for dealing with turbulent combustion, however, LES of partially-premixed combustion still constitutes an open challenge. To date, significant efforts have been done to develop turbulent combustion models for partially-premixed flame and some recent literatures can be found on modelling of partially-premixed flame with inhomogeneous inlets [6,7]. Tabulation techniques provide an advantage to calculate turbulent flame which include detailed chemistry at reduced computational cost. Bykov and Maas proposed a tabulation scheme called the reaction-diffusion manifold (REDIM) technique [8], which is the extension of intrinsic low-dimensional manifold (ILDM) method. REDIM method takes full account of the molecule diffusion process unlike ILDM method. This technique has been successfully used for premixed flame [9], stratified flame [10] and non-premixed flame [11]. This shows the generality of this method, which is not restricted to limited flame cases of premixed, non-premixed and partially premixed flames.

Present study uses reaction-diffusion manifold (REDIM) technique in combination with presumed filtered density function (PFDF) method to calculate turbulent partially-premixed flame cases, which have been jointly measured by University of Sydney and Sandia National Laboratory. PFDF methods are generally classified according to the shape of Filtered Density Function (FDF). Clipped Gaussian, top-hat and beta function are commonly used FDF shapes in LES. Present paper is focused upon top-hat FDF instead of ubiquitous beta FDF, as it is more suitable option to deal with multi-stream mixing problem.

2 REDIM-PFDF Combustion model

The REDIM chemistry table is obtained via the solution of an evolution equation for a low-dimensional manifold in the thermo-kinetic space:

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$$\frac{\partial \psi}{\partial t} = \left(I - \psi_\theta \psi_\theta^{+}\right)\left\{F(\psi) + \frac{d}{\rho}\chi \circ \psi_{\theta\theta} \circ \chi\right\} \tag{1}$$

The thermo-kinetic space is described by a vector $\mathbf{\Psi}$, which is a function of one or multiple reduced coordinates, given by the vector $\boldsymbol{\theta}$. The variable $\boldsymbol{\rho}$ is density, $\boldsymbol{\chi}$ is the vector of spatial gradient estimates for $\boldsymbol{\theta}$, $\mathbf{F(\Psi)}$ is the vector of the chemical source terms, $\mathbf{\Psi_\theta}$ is the matrix of partial derivatives of $\mathbf{\Psi}$ with respect to $\boldsymbol{\theta}$ and ψ_θ^{+} is its Moore-Penrose pseudo-inverse, $\mathbf{\Psi_{\theta\theta}}$ is the Hessian matrix. The symbol '∘' in Eq. 1 is an abbreviation for the multiplication of two vectors with a tensor of third order.

An initial guess and χ estimates need to be specified before the REDIM evolution equation can be calculated. It is observed that initial guess does not affect the solution, however, a good initial guess provides a fast convergence of the evolution equation. Similarly, it has been observed by Bykov and Mass, see e.g., [8],[9], that the REDIMs are not very sensitive with respect to χ and, with higher dimensional manifold its dependence on gradient becomes weaker.

Within the REDIM any number of reduced coordinates can be used, however, present case deals with multi-stream mixing problem so two reduced coordinates, i.e., mass fraction of CO_2 (Y_{CO2}) and mass fraction of N_2 (Y_{N2}) are used. Here Y_{CO2} and Y_{N2} represent reaction progress and mixing, respectively. All other species, density, temperature as well as production rate of CO_2 and so on, can be determined from the lookup table.

In LES of turbulent combustion governing equations are solved for filtered quantities and the filtered thermo-chemical quantities are modelled by the PFDF to approximate the flame structure at sub-grid scale

$$\tilde{f} = \int_{Y_{1,\min}}^{Y_{1,\max}} \int_{Y_{2,\min}}^{Y_{2,\max}} f(Y_1, Y_2)\, \tilde{P}(Y_1)\, \tilde{P}(Y_2)\, dY_1\, dY_2 \tag{2}$$

where P(Y_{CO2}, Y_{N2}) is the joint FDF. Under the assumption of statistical independence of Y_{CO2} and Y_{N2} the joint FDF can be written as the product of the two marginal FDFs, i.e. $\tilde{P}(Y_{CO2}, Y_{N2}) = \tilde{P}(Y_{CO2})\tilde{P}(Y_{N2})$. In this work, $\tilde{P}(Y_{CO2})$ is presumed to be Clipped Gaussian FDF, while $\tilde{P}(Y_{N2})$ is presumed to be top-hat distribution.

In the PFDF method, shape of the FDF is parametrized in terms of mean and variance of the variable. So both $\tilde{P}(Y_{CO2})$ and $\tilde{P}(Y_{N2})$ are determined by the mean and the variance, i.e., $(\widetilde{Y}_{CO2}, \widetilde{Y}''_{CO2})$ and $(\widetilde{Y}_{N2}, \widetilde{Y}''_{N2})$, respectively. In order to calculate the mean value additional transport equations for Y_{CO2} and Y_{N2} are solved with continuity and momentum equations. While the variance is modeled algebraically. The Favre filtered transport equation for mass fraction:

$$\frac{\partial \bar{\rho}\,\widetilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i}(\bar{\rho}\,\tilde{u}_i\,\widetilde{Y}_k) + \frac{\partial}{\partial x_i}(\overline{\rho\, u_i\, Y_k} - \bar{\rho}\,\tilde{u}_i\,\widetilde{Y}_k) = \frac{\partial}{\partial x_i}(\bar{\rho}\,\bar{D}\,\frac{\partial \widetilde{Y}_k}{\partial x_i}) + \bar{\rho}\,\tilde{\dot{\omega}}_k \tag{3}$$

where the index k =1, 2 denotes CO_2 and N_2, respectively. Note that for N_2 the source term ($\widetilde{\omega_k}$) in Eq. 3 is zero. The Favre filtered production rate is determined from the pre-calculated REDIM/FDF table employing the FDF method.

3 Experimental Setup

University of Sydney and Sandia National Laboratory jointly performed a series of experiments on a novel designed burner, as shown in Fig. 1 (left) to study behavior of turbulent partially premixed flame. This burner consists of two concentric pipes surrounded by a pilot with an inside diameter of D_3 = 18 mm and wall thickness of 0.2 mm. The inner or central pipe, which can be retracted upstream of the burner exit plane, has an inside diameter of D_1 = 4.0 mm and wall thickness of 0.25 mm. The main outer pipe or annulus has an inside diameter of D_2 = 7.5 mm and wall thickness of 0.25 mm. This burner assembly is centrally kept in a square cross sectioned wind tunnel (25×25 cm), which is supplying a co-flowing air stream at a fixed velocity Uc=15m/s. The inner pipe is recessed by 75 mm. Therefore, this burner configuration will lead to a partially premixed combustion mode. In the present work, two flame cases are considered: FJ200-5GP-Lr75-103 (FJ103) and FA200-5GP-Lr75-45 (FA45). For case FJ103, fuel flows through inner pipe with bulk velocity 120.6 m/s and air flows through outer pipe with bulk velocity 107.2 m/s. On the other hand in the FA45 case, air flows through inner pipe and fuel flows through outer pipe with the bulk velocities 105.8 m/s and 23.5 m/s, respectively. Mixture of C_2H_2, H_2, CO_2, N_2 and air in proper proportions is used to obtain the pilot flame, which exactly matches the composition of stoichiometric CH_4/air.

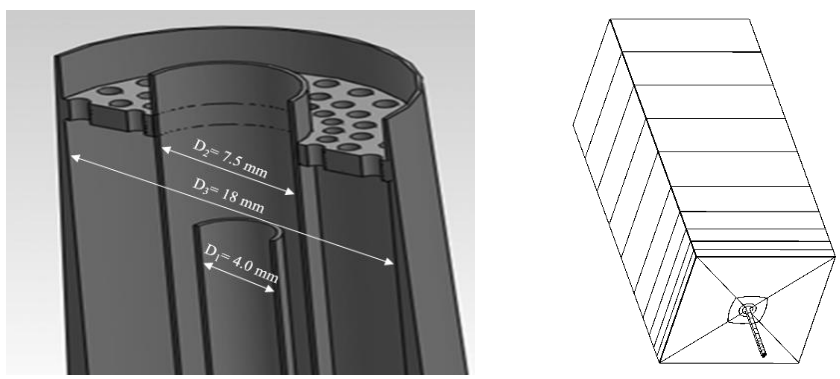

Figure 1. Left: schematic of the piloted turbulent burner with inhomogeneous inlets; right: global blocks of the computational domain

4 Numerical Setup

In the present study, REDIM-PFDF sub-grid model is implemented into the in-house finite-volume code LESOCC2C. The above code solves the Low-Mach number version of the compressible Navier-Stokes equations on body-fitted curvilinear block-structured grids using second-order central schemes in space and a three-step Runge-Kutta method of second order in time, and it is a robust code in dealing with turbulence combustion. The mesh used here is a body-fitted multi-block structured grid in which the whole computational domain is divided into 349 blocks and contains 5.25 million cells. In Fig. 1 (right), the solid lines show the boundaries of blocks. At the vicinity of the root of flame front the grid size is around 0.4, 0.2, 0.15 mm in axial, tangential and radial directions, respectively. A convective outflow boundary condition at the exit, and a uniform velocity profile without fluctuations at the inlet of the air-coflow and pilot flame inlet is applied. In order to obtain the fully developed turbulent flow, in the two pipes upstream of the inner pipe exit, a simulation of turbulent pipe flow with streamwise periodic condition is performed simultaneously.

4 Results & Discussion

Figure 2 explains the mixing pattern in both the flame cases. Figure 2 (left) shows the instantaneous snapshots of mixture fraction field for both the flame cases at the same time instance. For the FA45 flame case, uniform mixture fraction field is seen across the entire jet core near the jet exit plane. In contrast to the FA45 case, FJ103 flame case, shows high fuel concentration in the jet core near the jet exit plane and at farther downstream locations it shows uniform mixture fraction field

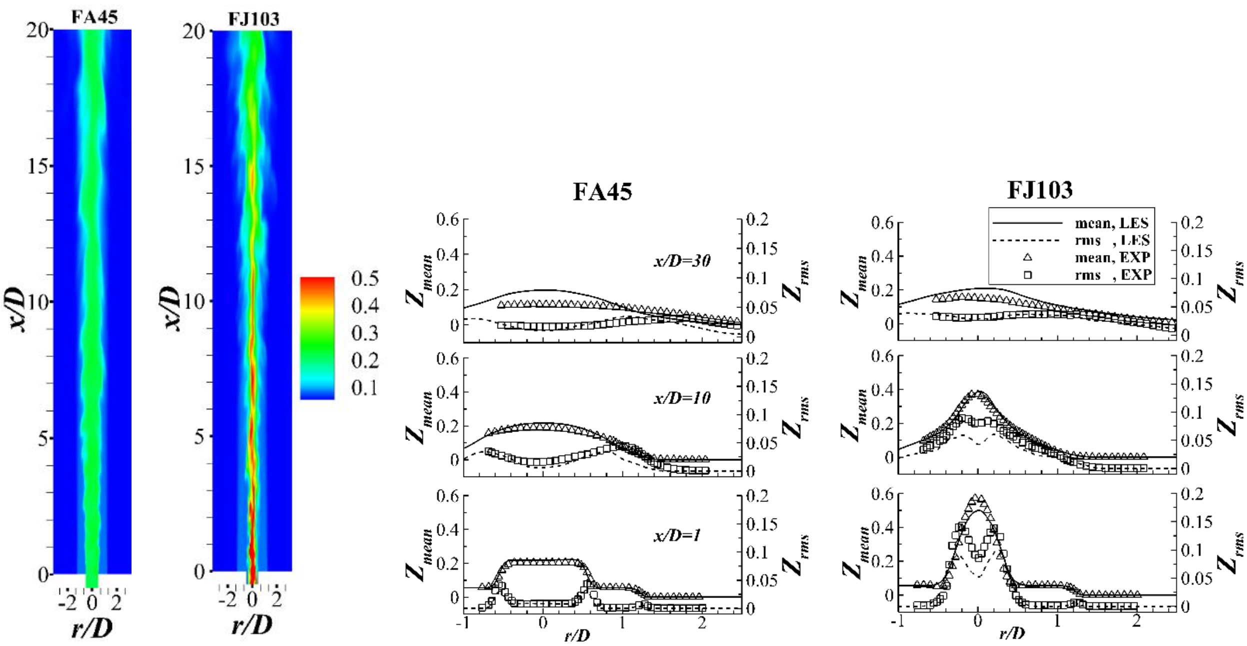

Figure 2. Left: Instantaneous snapshot of mixture fraction field at same time instance; right: comparison of calculated and experimental Favre mean and rms radial statistics of mixture fraction at different axial locations

Figure 2 (right) provides comparison of calculated and experimental Favre mean and rms radial statistics of mixture fraction at three different axial locations. It is clear that mixture fraction is predicted well by LES with REDIM-PFDF model for both the flame cases except at farther downstream location (x/D = 30), where Favre mean mixture fraction is slightly over-predicted by LES because of stronger spreading in the mixture fraction field. At x/D = 1, clear differences between mixing pattern of FA45 and FJ103 flame cases are seen. For the FA45 flame case, Favre mean mixture fraction shows top-hat profile near the jet exit plane with peak value Z_{mean} = 0.22. On the other hand, FJ103 flame case shows high mixture fraction gradient inside the main jet instead of the edge of the main jet. The Favre mean mixture fraction peak is at Z_{mean} = 0.48 for the FJ103 flame case, which is much higher than the FA45 flame case. Figure 3 and 4 provide flow field information at upstream locations and downstream locations, respectively. Figure 3 shows Favre mean and rms fluctuations of axial velocities, as well as shear stresses, $\overline{u'v'}$ calculated at different upstream locations. It is seen that both the flame cases show steeper gradient in the mean velocity at the edge of fuel and air stream near the exit plane (*x/D* = -9.8) and transformed into top-hat profile before entering into main chamber (*x/D* = -0.5), however peak value of mean velocity is higher in the FJ103 flame case than the FA45 case. Near the exit plane, the FA45 flame case exhibits higher shear stress value than the FJ103, which becomes flatter later for both the flame cases. This higher shear stress value causes intense mixing in the FA45 flame case, which is also observed in Fig. 2(right) where uniform mean mixture fraction is seen in the FA45 case at *x/D* = 1.

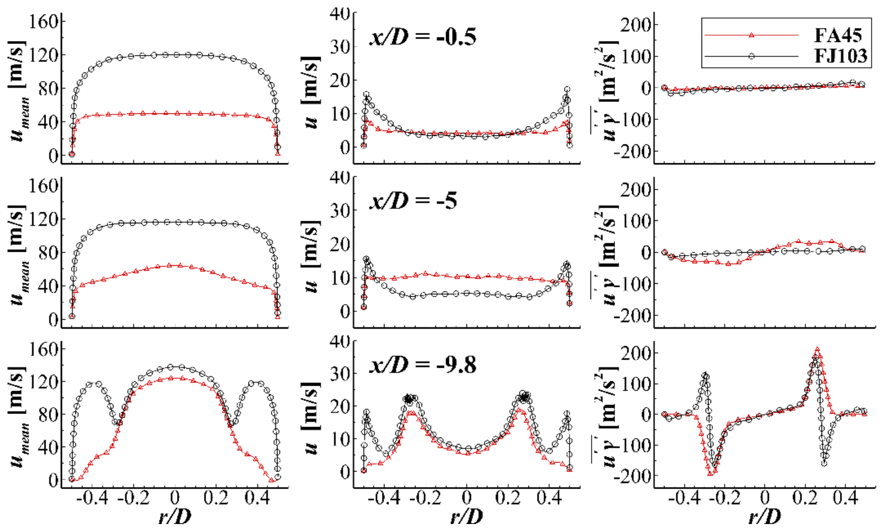

Figure 3. Favre mean and rms fluctuations of axial velocities, as well as shear stresses, $\overline{u'v'}$ calculated at different upstream locations

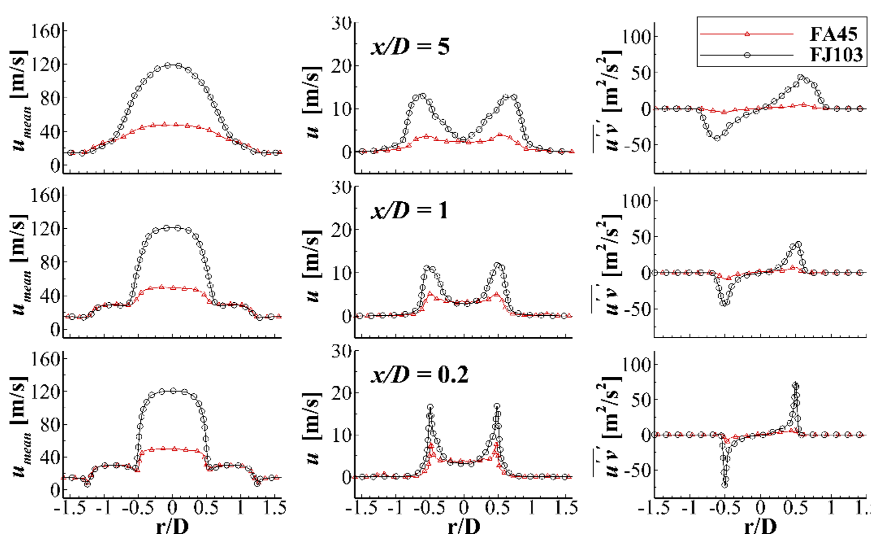

Figure 4. Favre mean and rms fluctuations of axial velocities, as well as shear stresses, $\overline{u'v'}$ calculated at different downstream locations

Favre mean and rms fluctuations of axial velocities, as well as shear stresses, $\overline{u'v'}$ calculated at different downstream locations are shown in Fig. 4. It is found that FJ103 flame case shows higher shear stress at the edge of the main jet near the exit plane because of larger velocity difference between the main jet and pilot flow than the FA45 case. It can be further seen that FJ103 case has a rapid spreading rate in the mean velocity than the FA45 case because higher turbulence levels near the edge of the jet cause more rapid entrainment of the pilot flow.

5 Conclusions

In the present work, two turbulent partially premixed flames have been simulated via LES with REDIM-PFDF sub-grid combustion model. Significant differences in the mean and rms fluctuations of the velocity and mixture fraction profiles are seen between the FA45 and FJ103 cases. The FA45 case exhibited near-homogenous mixture fraction field because of higher turbulence level at upstream locations, whereas FJ103 case is compositionally inhomogeneous near the jet exit plane. The overall agreement with the experimental data for mixture fraction field is satisfactory, which demonstrated the good performance of the REDIM-PFDF model in simulating partially premixed combustion.

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