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Assessment of Flame Structure of Turbulent Bluff-Body CH_4/H_2 Flame Using RANS-FPV Model

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Abstract - In this paper, numerical investigation of turbulent non-premixed bluff-body CH_4/H_2 flame using OpenFOAM-flamelet progress variable (FPV) has been presented. The work is based on the coupling of an in-house FPV solver with an OpenFOAM flow solver to investigate turbulent flames. Reynolds averaged Navier Stokes (RANS) based *k-ε* turbulence model in OpenFOAM was used to model the turbulent bluff-body flow. It was found that flow field characteristics such as predicted mixing field agreed well with the experimental data. For the CH_4/H_2 combustion, a detailed reaction mechanism was used, consisting of 32 species and 177 chemical reactions. Flamelet libraries were generated using an in-house flamelet solver for different scalar dissipation rates. PDF library was generated by invoking the information of mean mixture fraction, mixture fraction variance and progress variable from the flow solver. The predicted mean reactive scalars such as temperature and species mass fractions by the FPV model agreed well with the experimental data at all the axial locations.

Keywords**:** Turbulence-chemistry interactions, bluff-body flame, FPV model, OpenFOAM.

1. Introduction

The practical combustors such as domestic burner, industrial furnaces, power applications, and the transportation sector typically involve the generation of heat or power by burning fossil fuels. The combustion of fossil fuels will still play an essential role in global energy supplies in the decades to come. Since the last few decades, extensive focus has been made to design and develop combustion systems that would efficiently burn fuel and generate less pollutants. With the implementation of stringent emission regulations, various new combustion technologies, e.g., lean premixed prevaporised, homogeneous charged compression ignition, stratified charged compression ignition, etc., have been developed to reduce emissions. However, the implementation of new combustion technologies often pushes the combustion systems closer to their operating limits. In practical combustors, combustion occurs in a turbulent environment. There is a strong coupling between turbulence and combustion due to interaction between hydrodynamics of the flow and the heat release and species formation due to chemical reactions.

Over the last few decades, significant attention has been provided to model turbulent combustion using Reynolds averaged Navier Stokes (RANS) models and large eddy simulation (LES) based combustion models such as presumed PDF approaches such as flamelet [1], CMC [2] and the transported PDF [3]. These models have been used to study flame characteristics for several turbulent flames such as turbulent piloted, bluff-body, lifted flames [4-9]. Among these combustion models, the tabulated chemistry-based approach, i.e., flamelet model, is most attractive as there is a significant reduction of computational cost even with detailed chemistry. The flamelet concept was initially proposed for non-premixed flames by Peters [1]. It was found that the steady flamelet model unable to predict extinction and lift-off phenomenon in turbulent flames. This motivated Pierce and Moin [10] to develop a flamelet progress variable approach (FPV) to predict lift-off and extinctions in turbulent flames. Further, the ability of the FPV model to predict the local extinction and reignition phenomena in nonpremixed combustion was assessed by Ihme et al. [11] using DNS database. Ihme and Pitsch [12] used the FPV model to predict the NO formation and found reasonable agreement with the experimental data. Further, an unsteady FPV model was developed by Ihme and See [13] for the predictions of the autoignition phenomenon in turbulent lifted flames. Popp et al. [14] investigated the flame structure of partially premixed dimethyl-ether turbulent jet flame using the FPV model and found reasonable agreement with the experimental data.

Due to the advancement of computational power, the use of RANS and LES solvers for complex reacting flows have been increased substantially in the last decades. In this context, the importance of using robust open-source platform i.e., OpenFOAM [15] to investigate turbulent flames is increasing. OpenFOAM is an object-oriented C++ computational fluid dynamic tools and has the capability to solve problems related to heat transfer, laminar and turbulent flows, reacting flows, multiphase flows etc. Moreover, OpenFOAM provides a suitable platform to add advanced models, methods and numerical schemes which can be used in turbulence combustion research [16]. The implementation of the FPV model in the OpenFOAM would allow the combustion community to use RANS-FPV and LES-FPV models to investigate turbulent flames. Moreover, as OpenFOAM is composed of structured and unstructured meshing facilities and well-built MPI-based parallel algorithms, the coupled solvers may be used to solve practical combustors with complex geometry.

Hence, in this paper, the major objective is to model the turbulent reacting flow using OpenFOAM based flow solver and flamelet based combustion model, i.e., FPV model. RANS based turbulence model available in OpenFOAM will be used to model the turbulence flow field. The coupling process of the FPV solver with OpenFOAM will be validated against a turbulent bluff-body flame.

2. Flamelet Progress Variable Model

The flamelet concept was derived by Peters [1] for non-premixed flames. Flamelets are defined as thin reactive-diffusive layers embedded within a non-reactive turbulent flow field. According to this concept, the chemical time scale is very small compared to that of the convection and diffusion time scales. The steady flamelet equation is given as follows [1]

$$-\rho\frac{\chi}{2}\left(\frac{\partial^2\psi_\alpha}{\partial Z^2}\right)=\dot{\omega}_\alpha \tag{1}$$

where, ψ_α is any reactive scalar variable, $\dot{\omega}_\alpha$ is the reaction source term, Z is the mixture fraction space and χ is scalar dissipation rate which is given by [1],

$$\chi=2D\left(\frac{\partial Z}{\partial x_i}\right)^2 \tag{2}$$

For non-premixed combustion, scalar dissipation rate plays an important role. It represents the inverse of diffusion time scale and diffusion in mixture fraction space. The solution of steady-state laminar flamelet equations is tabulated in a two-dimensional library. The entries of this library consist of temperature and species mass fractions which are functions of Z and χ. If the form of PDF of Z and χ is known, then the mean value of reactive scalar quantities can be computed from

$$\psi_\alpha=\int_0^1\int_0^\infty\psi_\alpha(Z,\chi)\tilde{P}(Z,\chi)\,d\chi\,dZ \tag{3}$$

In the flamelet progress variable model, a new flamelet parameter λ, which is based on a reactive scalar has been introduced. The flame is then parameterized by the flamelet parameter rather than the scalar dissipation rate, which uniquely identifies each flame state along the S-shaped curve, including the unstable branch [10]. The flamelet parameter λ is defined through a reactive scalar *C (Progress Variable)*, which was introduced by Pierce and Moin [10] to be a linear combination of mass fraction of major reaction products, in this study CO_2, H_2O, and CO was used. The value of *C* can be found out by solving the transport equation as given below [10].

$$\frac{\partial\bar{\rho}\tilde{C}}{\partial t}+\frac{\partial(\bar{\rho}\tilde{u}_i\tilde{C})}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\bar{\rho}D\frac{\partial\tilde{C}}{\partial x_i}\right)+\dot{\omega}_c \tag{4}$$

The λ is assumed to be independent of mixture fraction and progress variable for given flamelet, and any reactive scalar can be expressed in terms of [10],

$$\psi = \psi(Z, C) \tag{5}$$

Mean values of the scalars can be determined by using the presume PDF approach, which is given by the below equation [[10]],

$$\tilde{\psi}_i = \int_0^1 \int_0^1 \psi_i(Z, C) \tilde{P}(Z, C) dZ dC \tag{6}$$

In Eq. 6 $\tilde{P}(Z, C)$ is the Favre joint PDF of Z and C. Using Bayes' theorem, the joint PDF is written in terms of a conditional PDF [[10]],

$$\tilde{P}(Z, C) = \tilde{P}(C \mid Z) \tilde{P}(Z) \tag{7}$$

Here $\tilde{P}(Z)$ was assumed to have a shape of β-PDF, and the conditional $\tilde{P}(C \mid Z)$ was estimated using δ-PDF . Similar to the transport equation of the mean progress variable, transport equations for mean mixture fraction and variance of mixtures were solved to obtain the PDF of mixture fraction.

3. Computational Details

In this section, computational details for the bluff-body flame and solution algorithm are described in details. The experimental data obtained by Dally et al. [17] for CH_4/H_2 bluff-body flame were used for modelling purpose in this study. Burner is centred in a coflowing stream of air and consists of a circular bluff body with an orifice at the center for the main fuel to enter [17]. The diameter of the bluff-body (D_b) is 50 mm, and that of the fuel jet is 3.6 mm. Fuel jet comprises of a CH_4/H_2 mixture by 1:1 volume ratio, coflow comprises of air. The bulk velocity of the fuel jet and coflow air are 118 m/s, and 40 m/s respectively. The temperature of fuel jet and coflow air is 298 K and stoichiometric mixture fraction Z_{st} is 0.05. Figure 1 shows the 2D schematic of the computational domain that was used in this work. The length of the computational domain is 7.2 D_b, and the width is 3 D_b. The number of control volumes selected was 72 and 144 in the x- and r- directions, respectively, based on the grid independence study.

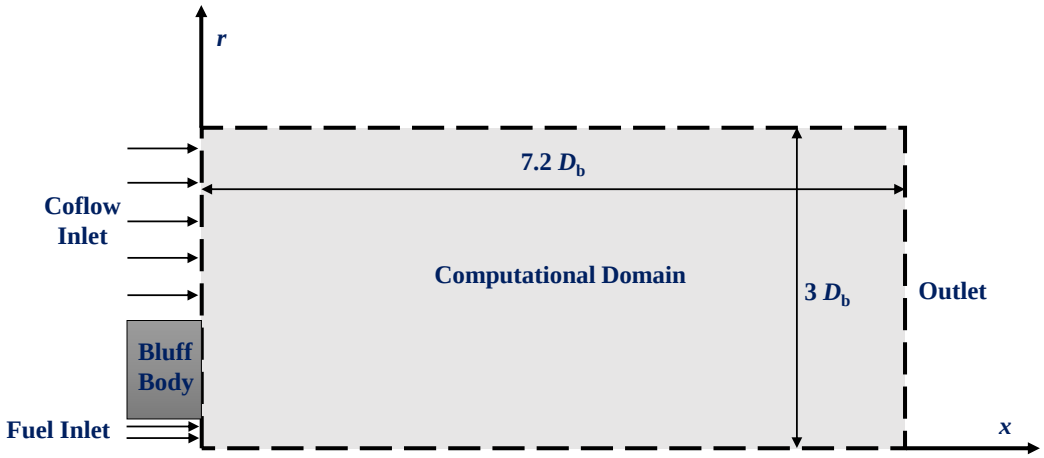

Fig. 1: Schematic of the non-premixed bluff body jet

The k-ε turbulence model was used to obtain the mean flow field. Transport equations for mean mixture fraction, variance of mixture fraction and mean progress variable were solved along with the flow solver. The reaction source term in the mean progress variable was updated using the flamelet table. Axis boundary condition was provided along the x-axis, whereas Neumann boundary condition was provided at the wall, top, and outlet face for all the variables. Pressure

outlet boundary condition was considered at the outlet. The coupling process of OpenFOAM flow solver and FPV model has been illustrated in Fig. 2. For the CH_4/H_2 combustion, a detailed reaction mechanism, GRIMech 1.2 [18] was used, consisting of 32 species and 177 chemical reactions. Flamelet libraries were generated using an in-house flamelet solver for different scalar dissipation rates. The PDF library was used to generate a lookup table in the flow solver. PDF library was generated by invoking the information of mean mixture fraction, mixture fraction variance and progress variable from the flow solver. The lookup table was called, and the mean reaction rate of the progress variable and density were updated in each time step in the flow solver.

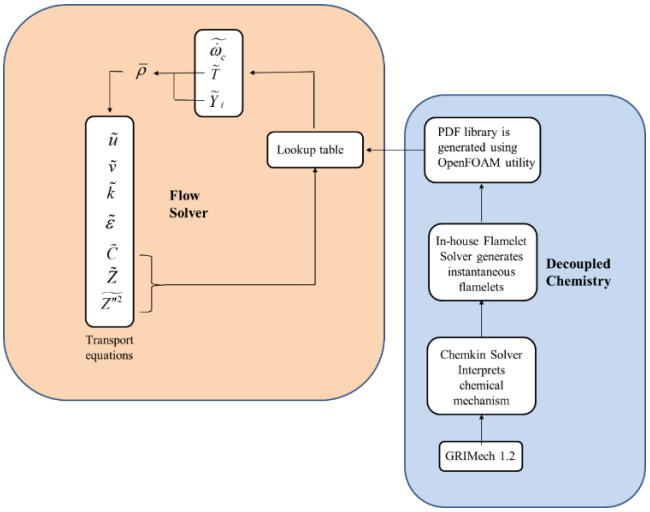

Fig. 2: Coupling of OpenFOAM and FPV solvers

4. Result & Discussion

In this section, results obtained for the mixture fraction, temperature and species mass fractions from the coupled solver are discussed.

The predicted mean mixture fraction by the flow solver is compared with the experimental data at three different axial locations, i.e., at x/D_b = 0.6, 0.9 and 1.8 and are shown in Fig. 3. The mixture fraction is a conserved scalar quantity, and it quantifies the process of mixing between fuel and oxidizer. For accurate predictions of the mixing field, the modelling constant $C_{\varepsilon 1}$ that arises in the k-ε turbulence model was modified from 1.44 and 1.6 to compensate for excessive dissipation [7] and is referred as MKE model. The trend of predictions obtained by the MKE agreed very well with the experimental data. At axial location x/D_b = 0.6, there is an excellent agreement with the experimental data; however, minor underpredictions are observed at the downstream locations. Higher-order RANS based turbulence model or LES models may be used to overcome these discrepancies.

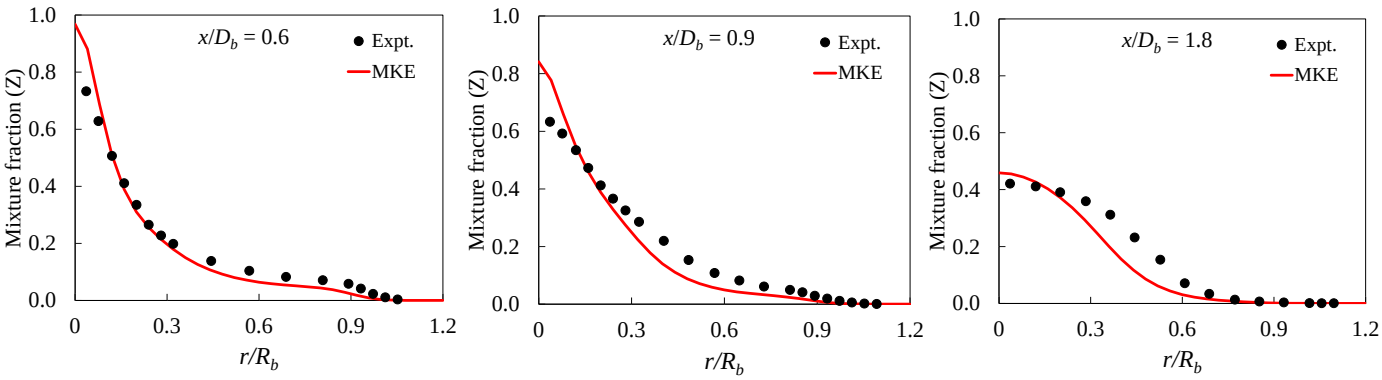

Fig. 3: Comparison of predicted radial mean mixture fraction with the experimental data at three different axial locations

Figure 4 shows the comparison of predicted radial mean temperature profile with the experimental data at three different axial locations, i.e., at x/D_b = 0.6, 0.9 and 1.8. The r.m.s values are provided on each experimental data of radial profiles of scalar fields. In the bluff-body burner, the flame gets stabilized just downstream of the bluff-body due to the presence of the recirculation zone, which lies between $0.26 < x/D_b < 0.9$. However, beyond the recirculation zone lies the neck region, i.e., between axial locations of $0.9 < x/D_b < 1.8$, where most activities like local extinction and reignition happen and are more intense at a higher level of turbulence. The trend of predicted mean temperature agrees well with the experimental data in the recirculation zone i.e., at x/D_b = 0.6 and 0.9 and in the neck region, i.e., at x/D_b = 1.8.

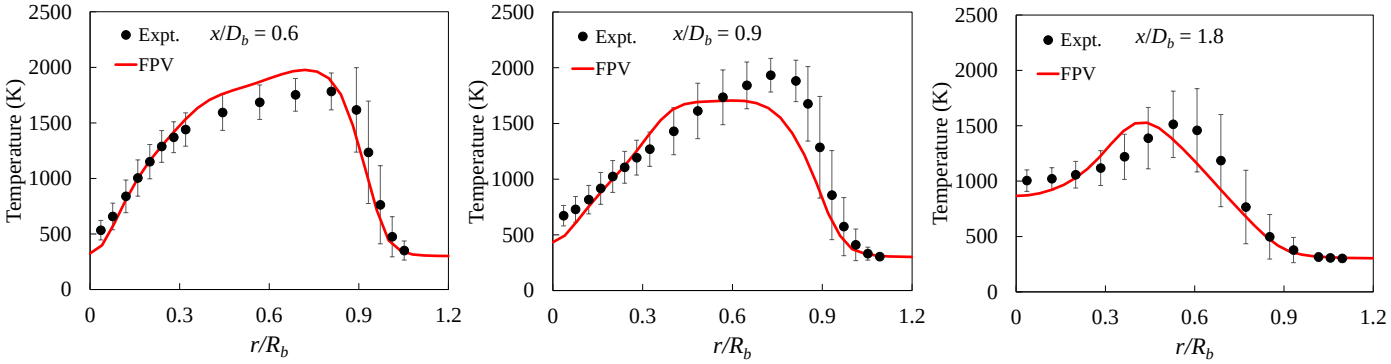

Fig. 4: Comparison of predicted radial mean temperature with the experimental data at three different axial locations

Figures 5 and 6 show the comparison of predicted radial mean H2O and CO2 mass fraction profile with the experimental data at three different axial locations, respectively. The predicted profiles of H2O and CO2 mass fraction matches very well with experimental data at x/Db = 0.6. Whereas at axial location x/Db = 0.9 for $0.4 < r/Rb < 0.9$ there is underprediction of H2O and CO2 mass fractions. A similar trend of underpredictions was also observed in the mixture fraction field at x/Db = 0.9. Mean reactive scalars such as temperature and species mass fractions were obtained by integrating the FPV solutions with PDF of mixture fraction and progress variable. Hence, any discrepancies in the predictions of mixture fraction will be lead to inaccurate predictions of the reactive field.

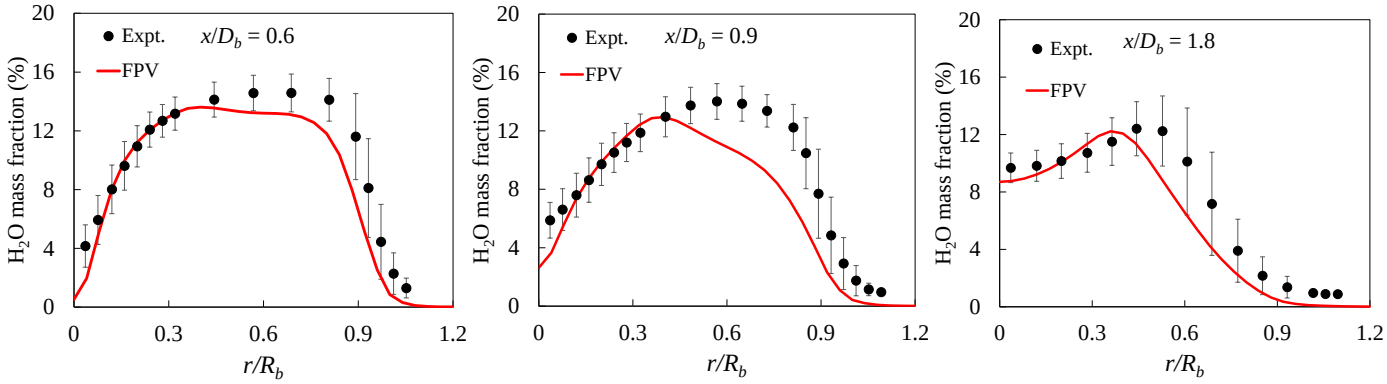

Fig. 5: Comparison of predicted radial mean H_2O mass fractions with the experimental data at three different axial locations

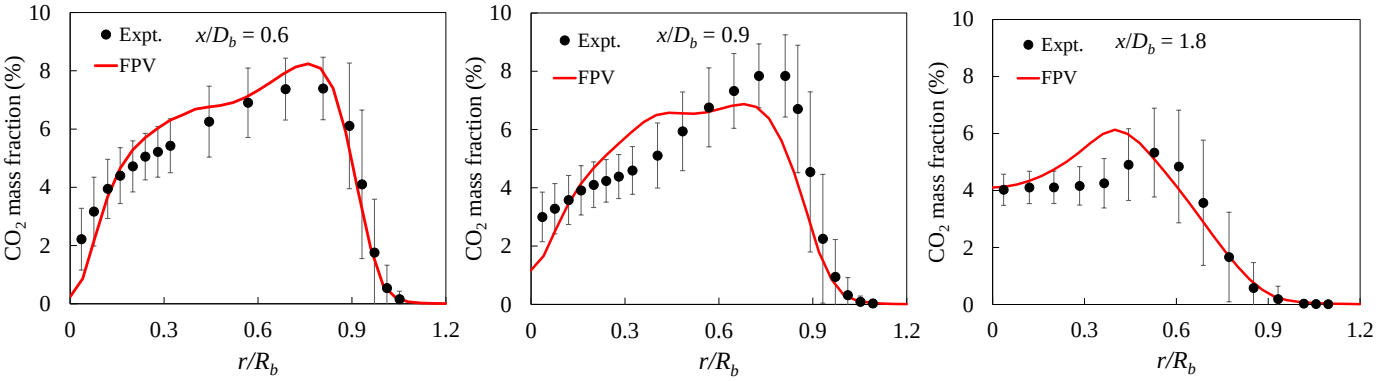

Fig. 6: Comparison of predicted radial mean CO_2 mass fractions with the experimental data at three different axial locations

5. Conclusion

In this work, a coupling of OpenFOAM flow solver and FPV combustion solver was attempted, and the coupled solver was used to predict the flame structure of a turbulent bluff-body CH_4/H_2 flame. RANS based turbulence model was used to predict the turbulent flow structure over a bluff-body. Predictions of mixing field, i.e., mixture fraction, agreed well with the experimental data while using MKE turbulent model where the modelling constant $C_{\varepsilon 1}$ that arises in the k-ε turbulence model was modified from 1.44 and 1.6 to compensate for excess diffusion. The temperature and species mass fractions were predicted very well with the coupled OpenFOAM-FPV model; however, improvement in the predictions of mixing field is required at few axial locations, which may further improve the predictions of reactive scalars. As the mean scalar quantities such as temperature and species mass fractions were obtained by averaging the flamelet solutions with PDF of mixture fractions and progress variable, higher-order turbulence models or large eddy simulation may be used to improve the predictions of the mixing field. The coupled OpenFOAM-FPV model in the present study has the potential to investigate the various phenomena arising in the turbulent flames.

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