Numerical Implementation and validation of turbulent premixed combustion model for lean mixtures

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Abstract. The present paper discusses the numerical investigation of turbulent premixed flames under lean conditions. Lean premixed combustion, a low NOx emission technique but are prone to instabilities, extinction and blow out. Such flames are influenced by preferential diffusion due to different mass diffusivities of reactants and difference between heat and mass diffusivities in the reaction zone. In this numerical study, we estimate non-reacting flow characteristics with implementation of an Algebraic Flame Surface Wrinkling Model (AFSW) in the open source CFD code OpenFOAM. In these flows, the mean velocity fields and recirculation zones were captured reasonably well by the RANS standard k-epsilon turbulence model. The simulated turbulent velocity is in good agreement with experiments in the shear-generated turbulence layer. The reacting flow study was done at three equivalence ratios of 0.43, 0.5 and 0.56 to gauge the ability of numerical model to predict combustion quantities. At equivalence ratios 0.5 and 0.56 the simulations showed numerical oscillations and non-convergence of the turbulent quantities. This leads to a detailed parametric variation study where, the pre-constant of AFSW model is varied with values 0.3, 0.35 and 0.4. However the study revealed the weak dependence of pre-constant value on the equivalence ratio. Hence the pre-constant value is fit for specific equivalence ratio based on the parametric variation study. The tuned AFSW model with fitted pre-constant specific to given equivalence ratio predicted are compared with experiments and discussed. The tuned AFSW model produced turbulent flame speed values which are good agreement with experiments.

1. Introduction

The study of premixed turbulent combustion is important to make the combustion more efficient and less harmful for nature. The research work focuses on the behaviour of lean turbulent premixed flame at high pressures. A well compiled large set of experimental data is available for validation. This data is chosen since the two main quantities of turbulent premixed combustion, turbulent flame speed (S_T) and flame brush thickness (δ_T) have been measured successfully. The specific objective of the current study is to make contribution in the field of numerical modelling of turbulent premixed combustion by implementing and validating a universal combustion model. The numerical simulations are carried out using RANS approach for modelling turbulence and laminar flamelet approach for modelling premixed combustion. The laminar flamelet modelling assumes that combustion happens in thin reaction zone regimes wherein the flame locally behaves as a laminar flame and turbulent flow structures are much bigger than combustion mechanism structures; hence the effect of turbulence on combustion is to wrinkle the local laminar flame and thereby enhance the combustion through increased flame surface area. The numerical simulations are carried out using open source CFD tool OpenFOAM solver.

A large set of well compiled experimental results have been produced through experiments carried out at Paul Scherrer Institute (Baden), Switzerland [1, 2, and 3]. The premixed turbulent flame is studied in a high-pressure combustion test rig (shown in figure 1, below) that is designed for a maximum operating pressure of 30 bars and a maximum air flow rate of 750m^3/hr. The combustion air/fuel mixture can be preheated up to 823K with an electrical heater. The study highlighted characteristics of non-reacting turbulent flow field and typical high-pressure turbulent premixed flame. The PIV measurements of flow field and planar Laser Induced fluorescence of OH radical distribution were used. The operating conditions for non-reacting flows (293K, 1bar) and for reacting flows a preheating temperature of 673K, pressures up to 14.44 bar (absolute), an equivalence ratio in the range ϕ=0.43–0.56 of premixed methane/air mixture at bulk flow velocity of 40 m/s. The turbulent intensity and integral length scale in the inlet are controlled using turbulence grid which is defined by hole diameter, blockage ratio and the axial position of turbulence grid within the combustor inlet section (see figure1). (for more details refer to Griebel et al. (2006)

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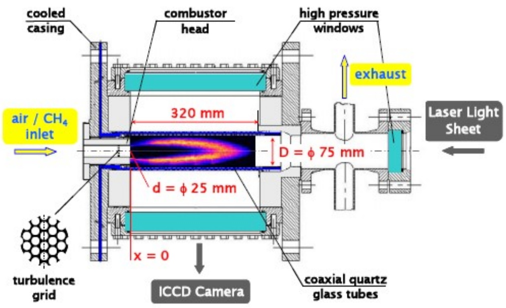

Fig 1. The experimental setup by Griebel et al. (2006)

2. Numerical Setup

The computational domain of combustion chamber used for all numerical simulations in this study consists of two co-axial cylinders of diameters 25mm which is a pre-inlet pipe and combustion chamber of diameter 75mm. The pre-inlet pipe of 25mm diameter goes for a length of 30mm serving two purposes. First, helps in letting the homogeneous turbulence flow enter the combustion chamber and second, creates a sudden expansion leading to recirculation zone which stabilises the flame. The combustion chamber of 75mm diameter goes for length of 320mm. The figure 2 below shows the schematic diagram of the computational domain considered.

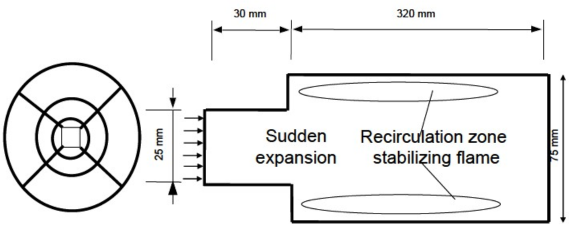

Fig. 2. The problem domain of High Pressure combustion chamber, (all dimensions in mm)

The computational grid for the above domain is created using ICEM [Ansys, Inc]. The grid independency test is carried out using two grids consisting of 300,000 cells and 600,000 cells. The grid with 600,000 cells is found to be adequate and all further reacting and non-reacting flow study is carried out using 600,000 cells grid.

3. Combustion Model

SPR Muppala (2005) model is a premixed turbulent combustion model which can be applied for different fuels up to pressure of 1MPa. Here the reaction source term of the reaction progress variable is modelled using laminar flame speed, corrected for stretch effects and turbulent flame surface area. The calculation of turbulent flame surface area is through a parameter called the flame-wrinkling ratio A_T/A . Flame wrinkling ratio is modelled with an algebraic parameterized relation. This term flame wrinkling ratio A_T/A is equivalent to turbulence flame wrinkling Ξ in Weller's Flame Area Combustion model [4]. The AFSW model is incorporated as the algebraic relation to calculate turbulence flame wrinkling as shown below. This model has been validated against various experimental data successfully [6, 7]. The combustion source term is modelled as,

$$\Sigma = \frac{A_T}{A} = \frac{S_T}{S_{L0}} = 1 + a\,\mathrm{Re}_t^{0.25}\left(\frac{u'}{S_{L0}}\right)^{0.3}\left(\frac{p}{p_0}\right)^{0.2}$$

Here, `a' is called pre-constant with 0.46, this parameter is linked to Lewis number making it possible to study molecular effects of diffusion on combustion [7].

4. Results and discussion

Non-reacting flow: In the investigation of turbulent flow field characteristics of non-reacting flows, the approach has been to study grid independency and to choose the appropriate turbulence model. From the experiments it was not clearly understood the degree of turbulence level that can be used in numerical simulations. Hence a detailed numerical non-reacting flow study is carried to fix the proper turbulence level and turbulence model. The results have been presented in detail [8]. The discrepancy in the turbulent flow field prediction using two different grids, one with 300000 control volume cells and another with 600000 control volume cells is shown in figure 3. Clearly gird with 600000 cells showed a better match with the experiments.

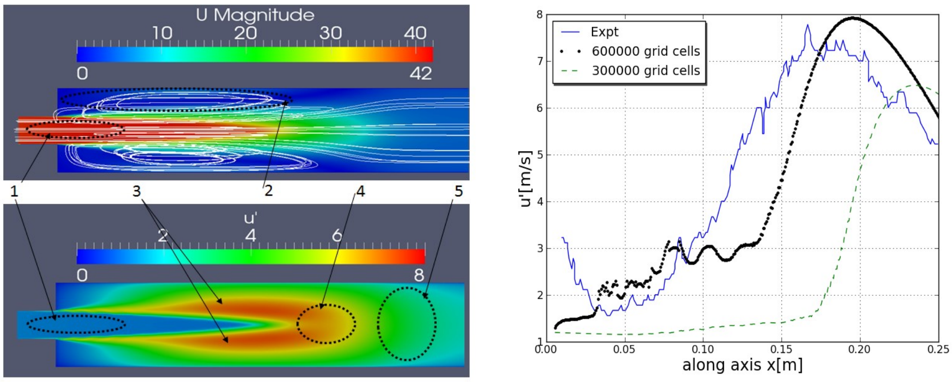

Fig. 3. Turbulent velocity u' along the axis of the combustion chamber for different grid cells with 5% turbulence level with the standard $k-\varepsilon$ turbulence model.

<u>Reacting flow study:</u> The RANS simulations were aimed at the study of behaviour of the turbulent premixed flames at different equivalence ratios, ϕ=0.43, 0.5 and 0.56. The flame characteristics like turbulent flame speed, flame position and flame brush thickness are measured and compared with experiments. The measurement of the flame length is the length along the axis of combustion chamber from start of the combustion chamber to the point where the value combustion regress variable is 0.5. The flame brush thickness is the distance along the axis of combustion chamber between the value combustion regress variable 0.05 to 0.95.

For ϕ=0.43: In the simulation study of turbulent premixed flames at varied equivalence ratios, the leanest mixture simulated was equivalence ratio φ=0.43. When such a lean mixture is under study low burning rates occur due to lower fuel concentrations. Under such lean conditions the flame is very sensitive to local flow changes or variations. The flame temperatures attained are low and combustion reaction happens to be an elongated long flame. The fig 3 gives contour plot of the reaction regress variable. The contour shows that a smooth elongated flame has been obtained, where the reactants indicated by colour red is getting burnt along flame (where the colour is changing from red to blue). The rest of the domain is covered by products (which is coloured in blue).

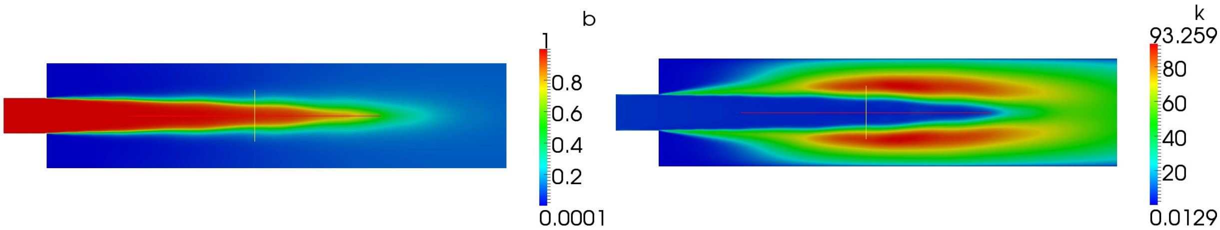

Fig 4. `b' regress variable contour and 'k' turbulent kinetic energy contour for equivalence ratio 0.43 using AFSW combustion model with original pre-constant. *Colour convention* blue (b=0) is burnt or combustion gas and red (b=1) is un-burnt or inlet premixed gas with 0<b<1.

The quantitative comparisons of the flame parameters predicted by the simulation and experimental values have been shown in the table. The current model under-predicts flame position in relative to the experimental flame position. While the turbulent flame brush thickness is over predicted, the flame temperature values are in good agreement with theoretical adiabatic flame temperature values.

For ϕ=0.5: Due to lower equivalence ratio resulting in lower chemical burning rate in the previous case of simulation discussed, the chemical reaction zone predominantly prevails far downstream of the domain. The increment in the equivalence ratio from 0.43 to 0.5 leads to higher chemical burning rate leading to the propagation of chemical reaction zone towards the upstream of the domain. The density drop across the flame due to combustion causes an expansion wave in the flow. The flame obtained is more corrugated and short due to turbulent structures and chemistry influencing each other. The flame possesses a long flame brush thickness almost of the order of the flame length itself.

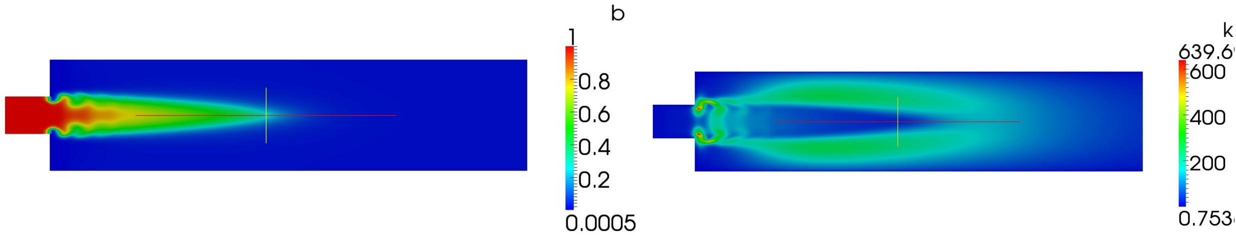

Fig 5. `b' regress variable contour and `k' turbulent kinetic energy contour for equivalence ratio 0.5 using AFSW combustion model with original pre-constant. Colour convention blue (b=0) is burnt or combustion gas and red (b=1) is un-burnt or inlet premixed gas with 0<b<1.

Turbulent flow field interaction with combustion is found to be very significant at equivalence ratio 0.5. Hence turbulence kinetic energy field did not converge even after 25 sweeps of domain. The turbulent kinetic energy contour shown below in figure 4 confirms the very non-uniform turbulent flow field.

For *ϕ=0.56*: The equivalence ratio has significant effect on the flame position and shape. The flame tends to shorten its length as the equivalence ratio is increased. The shape of the flame corresponds to the flame surface area. It is known from the fundamentals of chemical kinetics that, the rate of a reaction is directly proportional to the concentration of the reactants. Therefore at higher equivalence ratios the chemical burning rate increases due to higher fuel concentrations

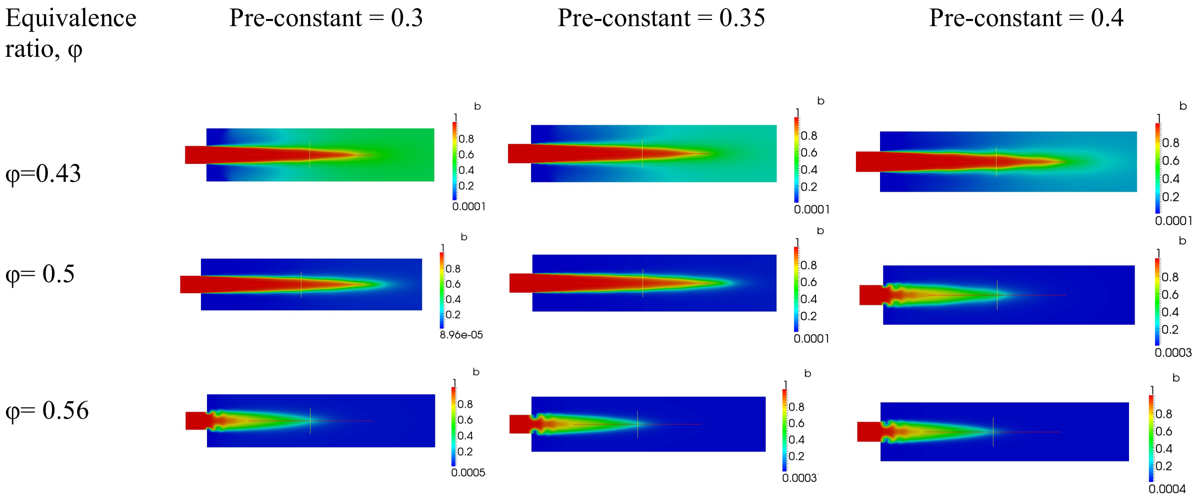

Fig 6. `b' regress variable contour and `U' mean flow velocity contour for equivalence ratio 0.56 using AFSW combustion model with original pre-constant.

resulting in the higher temperatures and higher turbulent burning velocities.

Colour convention blue (*b*=0) is burnt and *b*=1 indicates unburned. As a parametric variation study to mimic experiments the pre-constant parameter from its original constant of 0.46 for methane/air flames in the AFSW model is varied from 0.3 to 0.4. The pre-constant parameter value is varied to study the significance of this parameter on the flame stability and characteristics. The values are brought in to observe the change in chemical reaction rate prediction and its effect on the turbulence and combustion interaction to see if a converged solution can be obtained.

The above set of figures in the table gives complete idea of flame behaviour at different pre-constant values for the AFSW model. It is observed that the pre-constant value predominantly affects the chemical burning rate prediction. It is also observed that pre-constant value is weakly dependent on the equivalence ratio, because at equivalence ratio 0.43 the mixture does not burn completely as the pre-constant value is decreased. At the same time, the decrease in the pre-constant value brought converged solution at equivalence ratio 0.5. This indicates that a universal value of pre-constant cannot be used for all equivalence ratios.

Figure 6 shows the AFSW model over predicted the turbulent flame speed at equivalence ratio 0.43 whereas at equivalence ratio 0.5 and 0.56 predicted turbulent flame speed which is in good agreement with experiments. Turbulent flame speed is an important combustion parameter in study of combustion and the most difficult parameter to be able to predict by numerical models. The model showed no difference in flame lengths for all the equivalence ratios. Turbulent flame brush thickness is also in good agreement with experiments.

5. Conclusions

The study focused on the flow characterisation of the non-reacting and reacting flow field in the PSI high-pressure combustion test rig for methane/air lean mixtures. The operating conditions used are flow velocity of 40m/s, high pressure of 5bar and equivalence ratios of 0.43, 0.5 and 0.56. These conditions are mainly suitable for gas turbine power plants. An algebraic relation (AFSW model) for predicting the chemical burning rate in turbulent premixed flows has been implemented in the open source CFD code. The AFSW model is tested at various conditions to meet the experimental results through numerical simulations. The study suggested a need for fine-tuning of the model, hence a parametric variation study is carried out. This shows the pre-constant of AFSW model need to be tuned for each equivalence ratio which resulted in converged solutions. The tuned AFSW model predicted better turbulent flame speed and turbulent flame brush thickness values which are in good agreement with experiments. Further work is needed to achieve a universal relation valid for broad range of conditions.

References:

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