The effect of combustion sub-grid closures in LES of MILD combustion

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Introduction

In Moderate or Intense Low oxygen Dilution (MILD) [1, 2] combustion regime, the system evolves towards a distributed reaction regime and low temperatures, which leads to higher chemical and lower mixing time scales. Thus, the characteristic Damköhler number has the order of ∼1 [1, 2]. As a result, models accounting for finite rate chemistry should be considered. In the present work, the Partially Stirred Reactor (PaSR) model [3] is used. In PaSR, the influence of the sub-grid fluctuations on the reaction rate is expressed with a factor κ. Recently, it was shown that κ approaches 1.0 in MILD combustion, suggesting that reacting structures can be resolved on the Large Eddy Simulation (LES) grid using implicit models in which the turbulent effect is not directly included [4].

Methodology

The Partially Stirred Reactor (PaSR) [3] separates each computational cell into a reactive zone and a non-reactive zone [5]. The mean source term can be expressed as:

$$\overline{\dot{\omega}}_k = \kappa \dot{\omega}^*_k(\widetilde{\boldsymbol{Y}}, \widetilde{T}), \tag{1}$$

where $\dot{\omega}^*_k(\widetilde{\boldsymbol{Y}}, \widetilde{T})$ represents the formation rate of species k in the reactive zone based on the filtered mass fractions of species in the cell. The term κ is a coefficient which considers the effect from the non-reactive zone, calculated as: $\kappa = \tau_c/(\tau_c + \tau_{mix})$, where τ_c is the characteristic chemical time scale and τ_{mix} is the mixing time scale. Based on the PaSR model, the PaSR Quasi Laminar (PaSR-QL) model is formulated merely by forcing $\kappa = 1.0$ [6], under the hypothesis that the mixing time scale is much smaller than the chemical time scale. In the Finite Rate (FR) model, the mean formation rates are determined directly from Arrhenius expressions [7]. The PaSR-QL and FR models are defined as implicit combustion models because the influence of turbulence is not explicitly considered by including a mixing time scale τ_{mix}.

Experimental and numerical details

The Adelaide Jet in Hot Co-flow (AJHC) [8] burner has a central jet and an annulus pipe providing the hot co-flow with hot combustion products mixing with air and nitrogen. The hot co-flow has a mean temperature of 1300 K. The central jet provides an equi-molar mixture of CH_4 and H_2. In the present study, the condition corresponding to a Reynolds number of 10,000 and and co-flow oxygen content of 3% is studied. The open source CFD code of OpenFOAM is used for modelling. The whole domain is discretized with a 3D cylinder structured mesh containing ∼1.5 million cells. The one Equation Eddy Viscosity (oneEqEddy) model is chosen as the sub-grid scale model. A combustion solver based on PIMPLE algorithm with all three models (PaSR, FR, PaSR-QL) implemented is adopted. CFD time step is set to 2e-7 for the PaSR and PaSR-QL models and 5e-8 for FR. The KEE58 [9] mechanism is used to consider finite rate chemistry. The sampling locations are the centerline and 30/60/120 mm axial locations.

Results and discussion

The mean temperature profiles provided by the three combustion models are compared to the experimental data in Figure 1. The temperature profiles are similar, showing only minor differences between each other and very good predictions of experimental data. Regarding the centerline profile, the FR model corrects the slight over-prediction (around 7%) of mean temperature by the other two models. The rms value of temperature is shown in Figure 2. The first peak at axial 30 mm and 60 mm locations are well predicted by all

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the three models. Some under-predictions can be observed for the prediction of the second peak, indicating that the interaction between co-flow and air stream is under-estimated.

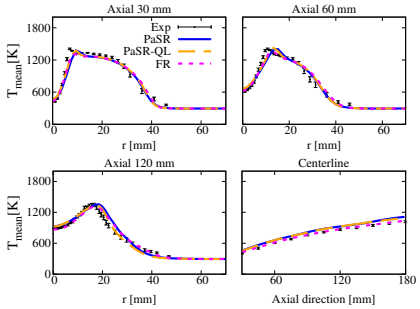

Figure 1: Mean temperature profiles.

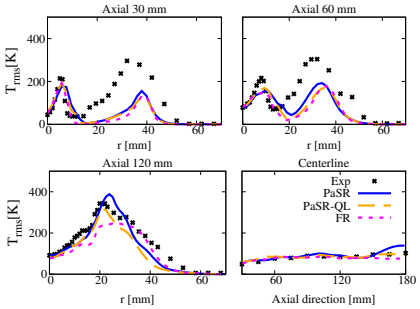

Figure 2: Root-mean-square (rms) temperature profiles.

In Figure 3, both the mean and rms value of CO are presented. The PaSR-QL model provides results very close to PaSR. The FR model slightly underestimates the mean CO peak value at z = 120 mm as well as the centerline profile.

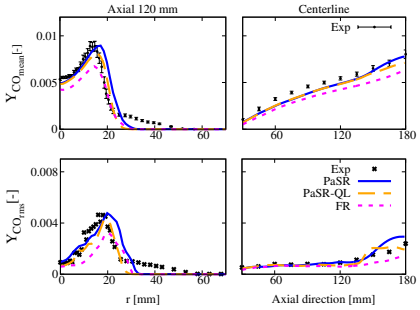

Figure 3: Mean and root-mean-square (rms) CO mass fraction profiles.

In order to assess the possibility of using implicit combustion models, the averaged values of κ obtained with the PaSR model are presented in Figure 4. It can be observed that, in the areas where combustion takes place (from z = 30 mm onward), κ values are in the range from 0.9 to 1.0, indicating that most of the cell is occupied by reacting structures.

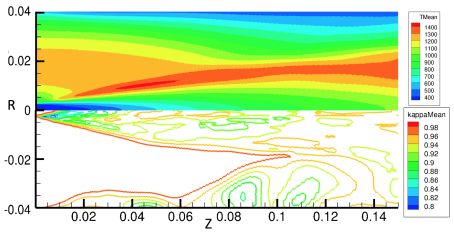

Figure 4: mean κ field (lower part) and mean temperature field (upper part) color map, axis unit: m.

Conclusion

The numerical results from the three models have demonstrated that the two implicit models have very similar behaviour compared with the conventional PaSR model and they all give satisfactory predictions, especially the mean values. Furthermore, the κ values are close to 1.0 on most locations with PaSR. This validates the usage of implicit combustion models in low Damköhler number (Da $\leqslant$ 1.0) systems.

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