LES of MILD combustion with adaptive finite rate chemistry

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Introduction

The present work focuses on the validation with OpenFOAM for the numerical simulation of turbulent combustion under Moderate or Intense Low-oxygen Dilution (MILD) combustion. Results for a Jet-in-Hot-Coflow (JHC) burner using a mixture of CH_4 and H_2 50/50 on molar basis[1] are presented and discussed. Simulations are performed using Eddy Dissipation Concept (EDC) combustion model combined with edcPimpleSMOKE, a transient solver coupled to the OpenSMOKE[2] tool for stiff chemistry management. The detailed kinetic mechanism KEE[3] is used for chemical reactions.

Methodology

For the first section of the simulation work, the Reynalds Averaged Navier-Stokes (RANS) simulation is conducted on a 2D mesh with 30,000 computational cells. The sensitivity of the results to different modelling parameters and numerical approach is investigated, with the objective of giving some preliminary references to the Large Eddy Simulation (LES) work. The sensitivity analysis approaches include the choice of the k-epsilon model parameters, the choice of canonical reactor simulating the fine structures and the EDC model coefficient[4][5]. Moreover, the impacts of molecular and turbulent diffusion on the results are assessed.

Next, based on the RANS set-up, a LES is carried out on a 3D cylinder mesh of 3 million cells. The Synthetic Turbulence inflow generator[6] is used to provide a transient velocity boundary condition.

Finally, there is a combination of EDC combustion model with $in-situ$ adaptive tabulation (ISAT)[7] and Direct Relation Graph (DRG)[8], both in RANS simulation and LES, in order to evaluate the potential of computational time reduction.

Results and Discussions

In this section, part of the sensitivity analysis work with RANS simulation is presented. In Fig. 1, the effect of the $C_{1\epsilon}$ constant in k-epsilon model is demonstrated,

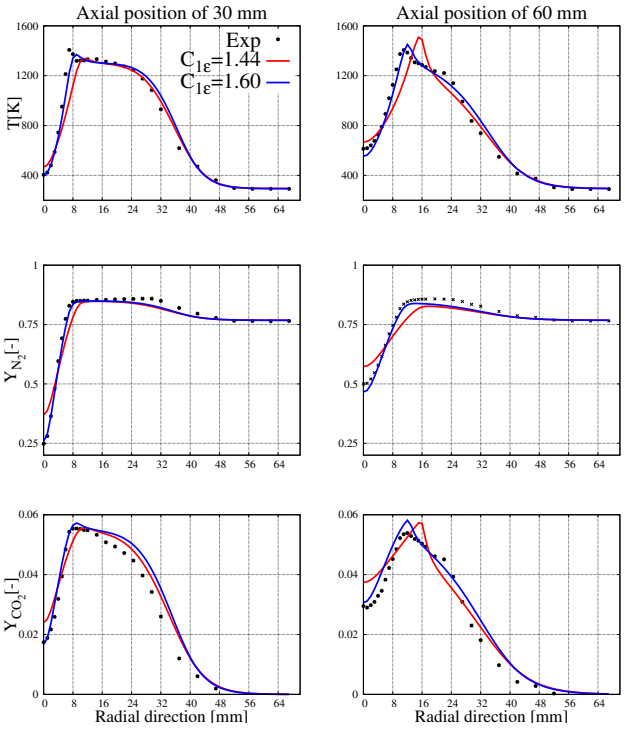

Figure 1: Simulation results of Temperature, Y_{N_2} and Y_{CO_2} profiles on the axial position of 30 mm and 60 mm downstream of the jet exit with differnt $C_{1\epsilon}$ value ($C_{1\epsilon} = 1.44$ and $C_{1\epsilon} = 1.60$) comparing with experimental profiles.

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in which Exp. represents the experimental data. The value of $C_{1\epsilon} = 1.44$ is the default one for most fluid dynamics applications, whereas here it is compared to $C_{1\epsilon} = 1.60$. From the plots in Fig. 1, it is obvious to see that with $C_{1\epsilon} = 1.60$, results closer to the experimental profiles can be achieved, especially when it is in the region close to the jet centerline (radial direction close to 0). The peak temperature position and value are better handled with $C_{1\epsilon} = 1.60$ as well. As a result, conclusion can be drawn that $C_{1\epsilon} = 1.60$ can give better profiles in most cases and thus it is more suitable for the current simulation work.

The effect of the turbulent Schmidt Number in the diffusion term of the species transport equation is also taken into account. With Schmidt Number equals to 1.0, 0.7 and 0.6, the impacts on species mass fraction of N_2, CO_2 and temperature predictions are presented in Fig. 2. Plots on the axial position of 30 mm show that with Schmidt Number equals to 0.7, the profiles near the jet centerline can be better predicted. On the axial position of 60 mm, Schmidt Number equals to 0.7 helps to correctly simulate the position and value of the peak temperature.

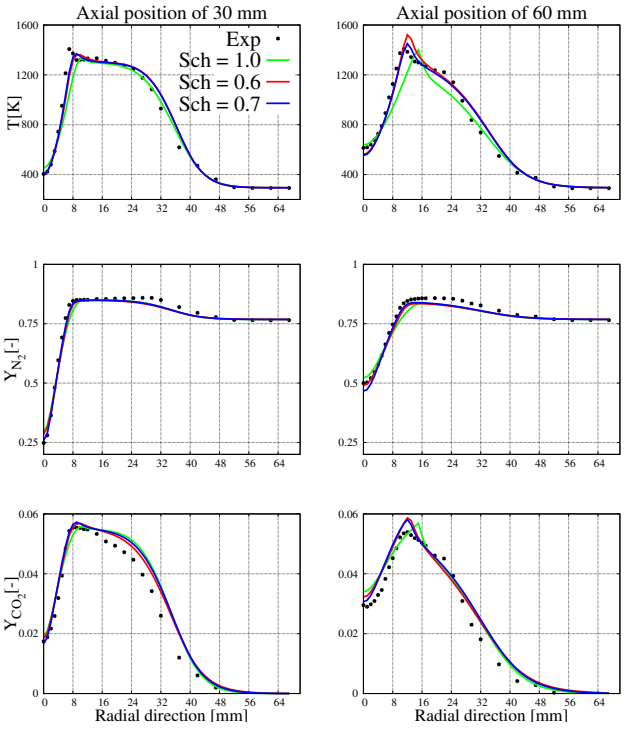

Figure 2: Simulation results of Temperature, Y_{N_2} and Y_{CO_2} profiles on the axial position of 30 mm and 60 mm downstream of the jet exit with differnt Schmidt Number value ($Sch = 1.0$, $Sch = 0.7$ and $Sch = 0.6$) comparing with experimental profile.

Conclusion

The present work reports on a sensitivity analysis carried out on a burner operating in MILD condition. Sensitivity analysis show that the modifications of the k-epsilon $C_{1\epsilon}$ constant to 1.60 and of Schmidt Number to 0.7 help to improve the prediction of the species mass fraction and temperature profiles. The usage of ISAT is able to save the computational time by 2 to 3 times with the tolerance set to 10^{-6}. In addition, the effect of chemistry reduction via DRG is being investigated in both RANS and LES frameworks.

Acknowledgments

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