LARGE EDDY SIMULATION OF A MULTI-REGIME BURNER USING VIRTUAL CHEMISTRY

Tan-Phong LUU, Nasser DARABIHA, Benoît FIORINA
EM2C-CNRS, CentraleSupélec, Université Paris-Saclay
91190, Gif-sur-Yvette, France

ABSTRACT

In order to build the next generation combustion chambers, numerical models must be able to accurately describe the multi-regime flame happening in practical applications. Pollutant formation in particular has been highlighted to be considerably different in multi-regime flames compared to canonical premixed or non-premixed flames. The objective of this work is to challenge an innovative chemistry reduction method called virtual chemistry to the Large Eddy Simulation (LES) of a multi-regime flame configuration. The novel Darmstadt multi-regime burner has been chosen providing a rigorous framework in which simulations can be performed and compared against measurements. The low-Mach YALES2 code using a thickened flame mode for the LES has been employed. Time-averaged experimental and numerical data of axial velocity, temperature and CO mass fraction are compared. Preliminary results show overall good correspondence with experiments near the exit burner, albeit improvement can be expected from a finer mesh and longer time-averaging.

Keywords : Reduced chemistry ; Turbulent combustion modeling ; Multi-regime combustion ; Large-Eddy Simulation ; CO formation

1 INTRODUCTION

Most of novel combustion chambers promote stratified combustion regimes to limit the flame temperature while ensuring the flame stabilization [1]. In terms of turbulent combustion modelling, challenges are to handle complex interactions between detailed chemistry effects and turbulence in both premixed and non-premixed combustion regimes [2]. While multi-regime combustion models have been developed during the last decades [3–7], several configurations have been designed in parallel to challenge their efficiency. One of the most studied configurations is the Sydney Inhomogeneous burner [8], which has been computed as a target flame within the TNF workshop [9]. New insights in turbulent combustion modelling resulted from numerous comparisons between simulations and experiments [10–15]. However, uncertainties in the main inhomogeneous jet and pilot stream boundary conditions limit the simulations accuracy.

Darmstadt combustion research group (University of Applied Sciences Darmstadt (h_da) and Technical University Darmstadt (TUDa)) has recently designed the multi-regime burner (MRB) [16] providing a

Correspondence to: tan-phong.luu@centralesupelec.fr

comprehensive experimental database including velocity, temperature and CO measurements for multi-regime combustion processes. Popp *et. al.* [17] performed the first LES of the MRB, using an artificial thickened flame approach coupled with premixed-based tabulated chemistry. The study showed that, due to strong effects of local transport phenomena, an additional transport equation for CO mass fraction significantly improves the model accuracy.

A new chemical reduction strategy, called virtual chemistry [18], has been developed to capture the chemical structure of multi-regime combustion. The methodology consists in designing a highly-reduced mechanism from scratch, instead of simplifying a detailed mechanism. The mechanism includes virtual species and virtual reactions whose thermodynamics and chemical properties are optimized using a machine learning algorithm to capture user-specified target flames quantities. A virtual main mechanism dedicated to capture the temperature and heat release [18] and a satellite sub-mechanism for CO prediction [19] have been first validated in both laminar premixed and non-premixed adiabatic configurations. The virtual model has been then coupled with the LES formalism by using a thickened flame approach [20] to compute non-adiabatic premixed swirled combustor [21] and the Sydney configuration [7].

The present work aims to challenge the virtual chemistry approach on the MRB configuration. A presentation of the experimental setup is first provided, followed by the numerical models and setup used. Then, preliminary results comparing measurements and simulated data are shown before concluding.

2 TURBULENT COMBUSTION MODEL

2.1 Combustion model : TFLES

A thickened flame approach is used in order to solve the chemical reactions happening in the flame front. This approach consists in artificially thickening the flame front by introducing a thickening factor F and an efficiency function E_Δ representing the flame wrinkling in the subgrid scale. As such, the diffusivity of the different species increases by $E_\Delta F$ whereas the production rate is multiplied by a factor E_Δ/F, modifying the LES species mass balance equation (Eq. 1) as follows:

$$\frac{\partial \tilde{\rho}\widetilde{Y_k}}{\partial t} + \nabla \cdot (\tilde{\rho}\tilde{\mathbf{u}}\widetilde{Y_k}) = -\nabla \cdot (E_\Delta F \overline{\rho \mathbf{V_k}}\widetilde{Y_k}) + \frac{E_\Delta}{F}\dot{\omega}_k(\widetilde{Q}) \tag{1}$$

where ρ is the density, Y_k the mass fraction of the k^{th} species, $\mathbf{u}$ the velocity vector, $\mathbf{V_k}$ the diffusion velocity of the k^{th} species, $\dot{\omega}_k$ the reaction rate of the k^{th} species with Q any quantity entering the computation of the reaction rate. In this equation $\overline{f}$ and $\widetilde{f}$ denote filtered and mass-weighted filtered of quantity f respectively. To close Eq. 1, the Charlette model [22] with Wang et al. correction [23] is used to compute the efficiency function E_Δ, with $\beta = 0.5$ (Eq. 2).

$$E_\Delta = \left(1 + \min\left[\frac{\Delta}{\delta_L^0} - 1, f\left(\frac{\Delta}{\delta_L^0}, \frac{u'_\Delta}{S_L^0}, Re_\Delta\right)\frac{u'_\Delta}{S_L^0}\right]\right)^\beta \tag{2}$$

where Δ is the filter size, δ_L^0 the laminar flame thickness, u'_Δ the sub-grid scale velocity fluctuation, S_L^0 the laminar flame speed, Re_Δ the sub-grid scale Reynolds number.

2.2 Chemistry model : Virtual chemistry

The virtual chemistry method [18, 19, 21] falls within the reduction of kinetic schemes. It consists of creating virtual species and reactions whose physical and chemical properties are optimized using a ma-

chine learning algorithm in order to retrieve key variables of interest. These variables are representative of canonical configurations, computed with an in-house solver [24].

The virtual scheme used in the present work is built using a reference database including both premixed and non-premixed 1-D CH4/air flames at 300 K and 1 atm. It consists of two blocks : a 2-step main mechanism (Eqs. 3 and 4), whose objective is to ensure the temperature evolution and the flame speed, and a 3-step satellite sub-mechanism (Eqs. 5, 6 and 7), optimized to retrieve carbon monoxide formation.

$$\alpha_F^v F + \alpha_{Ox}^v Ox \rightarrow \alpha_I^v I \tag{3}$$

$$\alpha_I^v I \rightarrow \sum_{k=1}^{4} \alpha_{P_k}^v P_k \tag{4}$$

$$\alpha_F^v F + \alpha_{Ox}^v Ox \rightarrow \alpha_{CO}^v CO + (1 - \alpha_{CO}^v) V_1 \tag{5}$$

$$F + V_1 \rightarrow F + CO \tag{6}$$

$$CO \leftrightarrow V_2 \tag{7}$$

In these reactions, F, Ox and CO represent fuel, oxidizer and carbon monoxide respectively. I is a virtual intermediate species producing 4 virtual products P_k. V_1 and V_2 represent virtual intermediate species producing CO.

3 STUDIED CONFIGURATION

3.1 Experimental configuration

The multi-regime burner (MRB) is detailed in [16]. A rich premixed flow of methane and air is injected through the center tube (called "jet") at a bulk velocity of $v_{jet} = 105$ m/s. The main injection is surrounded by two concentric annular tubes, called "slot 1" and "slot 2" respectively. An air flow is injected at $v_{slot1} = 15$ m/s through the first annular tube (slot 1). A lean ($\phi_{slot2} = 0.8$) premixed flow of methane/air is injected at $v_{slot2} = 20$ m/s through the second annular tube (slot 2). The temperature of the conical bluff body separating the annular tubes is regulated by water at 80 C. Finally, a second bluff body separates the "slot 2" and an air co-flow at $v_{coflow} = 1$ m/s. Two configurations of interest, differing by the equivalence ratio of the "jet" flow, have been studied by [16]. The configuration called MRB18b, corresponding to $\phi_{jet} = 1.8$, is the one simulated in the present work.

3.2 Numerical setup

The LES of the MRB18b configuration presented in this work has been performed using the unstructured finite-volume YALES2 code [25], with a low Mach number formulation. 4^{th}-order discretization schemes are used for spatial and temporal integration of the convective terms. The sub-grid scale turbulence is closed with the SIGMA model [26]. The cylindrical computational domain has a length of 1.6 m in the axis of the burner and a radius of 500 mm. The mesh is composed of 68 millions of tetrahedra, whose sizes expand along the axis of the burner from 0.1 mm near the burner exit, to 0.5 mm further downstream about where the flame stops, to 50 mm at the far end of the domain (about 1.1 m far from the exit of the burner). The size of the cells also expands radially, such that 0.1 mm $\leq \Delta_{cell} \leq 0.3$ mm in the inner reaction zone, and 0.4 mm $\leq \Delta_{cell} \leq 0.6$ mm in the outer reaction zone. Time-averaged data have been calculated over 5 flow-through times, taking the bulk velocity of the jet injection as reference.

4 PRELIMINARY RESULTS

Time-averaged mean experimental and numerical radial profiles of axial velocity, temperature and CO mass fraction are shown in Fig. 1 at three different heights from the burner exit.

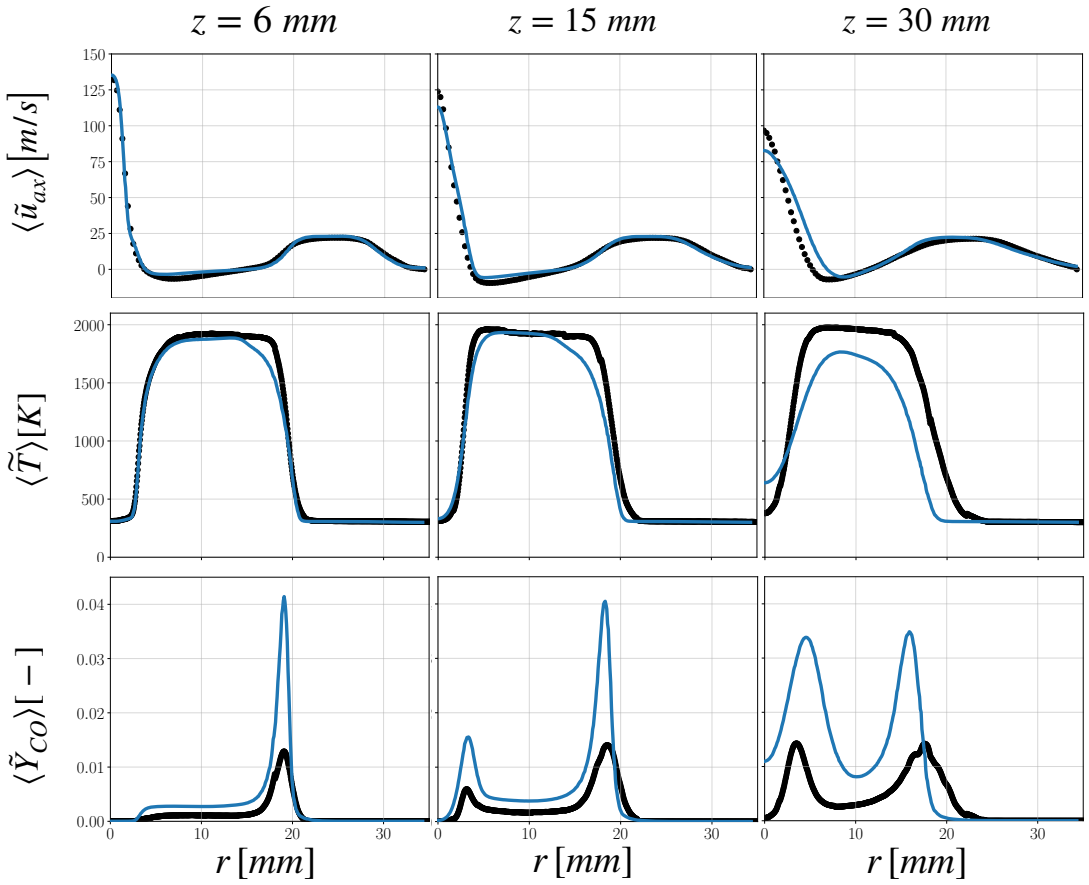

Figure 1: Mean radial profiles of axial velocity (top), temperature (middle) and CO mass fraction (bottom).

For all axial positions, a fair agreement is observed between mean numerical and experimental axial velocity. The mean temperature profile is also well predicted at $z = 6$ mm and $z = 15$ mm with however a slight discrepancy in the outer flame region (15 mm $< r <$ 20 mm). At $z = 30$ mm, a the difference between experimental and numerical data is more pronounced. Concerning the CO mass fraction, whereas the shape of the profiles is well captured, peaks are overpredicted in both inner and outer flame fronts.

These results are preliminary and will be further consolidated by first increasing the computational time retained for the statistics. Indeed, as described by [17], the presence of slow large-scale recirculating zones affects the time needed for the averaging. Second, the mesh will be refined in the flame region. In fact, as highlighted in Fig. 1, the numerical temperature profile experiencing a drop in the outer flame region and the flame being shifted towards the centerline could be explained by coarse cell size.

5 CONCLUSION

Using virtual chemistry methodology coupled with thickened-flame LES, the Darmstadt multi-regime burner has been simulated on a grid of 68 millions of tetrahedra with the low-Mach YALES2 code. Numerical radial profiles of the axial velocity temperature and CO mass fraction have been compared against experimental data and showed good overall agreement. However, far from the flame recirculating zones, discrepancies were observed. To improve the results' quality, ongoing work focuses on improving the statistical convergence and mesh refinement.

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