LES of the Jet-in-Hot-Coflow configuration without resorting to Turbulence Chemistry Interaction modeling

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Introduction

Diluted combustion systems constitute a promising way to reduce nitrogen oxides (NO_x) emissions, since they allow to reduce the temperature peak in the reaction zone. As a consequence, the reaction rates are lower compared to classic combustion. The Damköhler number Da, comparing the characteristic times of the turbulence and of the chemical kinetics, is such that $Da \approx 1$. Numerical simulation of such systems is particularly challenging as the Turbulence-Chemistry Interaction (TCI) and the Turbulence-Radiation Interaction (TRI) are key issues. The aim of this study is to assess the relevance of performing LES of diluted combustion without resorting to the TCI modeling. Large Eddy Simulations (LES), using Finite Rate Chemistry (FRC) combined with a skeletal reaction mechanism, were performed on the Jet-in-Hot-Coflow (JHC) [2].

Burner description

The design of the Jet-in-Hot-Coflow allows to approach diluted combustion conditions. The coflow, distributed in an annular zone around the fuel injection, results from an upstream combustion (Fig. 1). It is thus composed of a mixture with a low oxygen concentration and brings heat to reach a temperature above the self-ignition temperature of the fuel. For the Adelaide flame [2] analysed in this study, the coflow is at 1300 K and its composition is 6% O_2, 82% N_2, 6.5% H_2O, 5.5% CO_2, by mass. The fuel is enriched with hydrogen: 88% CH_4, 12% H_2, by mass.

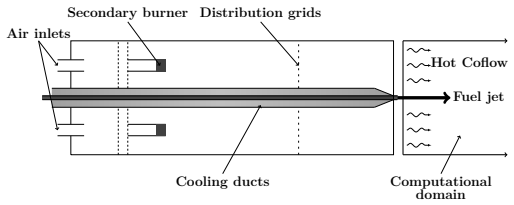

Figure 1: Sketch of the JHC burner.

Kinetic mechanism

Chemical kinetics simulations were preformed using the Cantera software [3] in order to choose the kinetic scheme. A 1D counterflow diffusion flame was simulated with the temperature and composition conditions of the studied flame. The skeletal mechanism DRM22 [4] was chosen as the profiles of the main quantities obtained with this scheme and with GRI-3.0 [5] overlay, see figure 2.

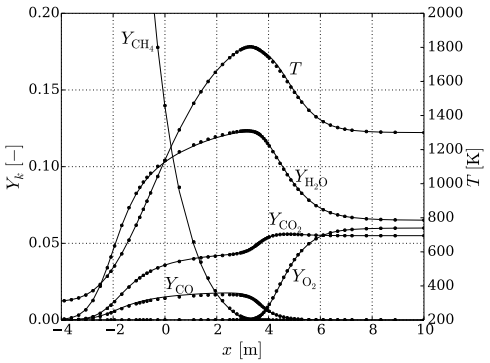

Figure 2: Species mass fractions and temperature in 1D counterflow diffusion flame using GRI-3.0 (•) and DRM22 (–).

Numerical setup

The domain has a cylindrical shape with a radius $R = 18\,D$, where D is the inner diameter of the injection, and an axial length $L = 62\,D$. The fuel and coflow injectors lengths are $6.7\,D$ and $3.35\,D$, respectively. The lips of the fuel injection are modeled as they have an impact on the shear layer between the fuel and the coflow. A convergent nozzle is added at the end of the domain to avoid back flow recirculations. The grid is build of 17.7 million tetrahedral cells and is refined in the flame region ($h \approx 400\,\mu$m). The boundary conditions imposed on the inlets are summarized in Tab. 1.

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	Fuel	Coflow	Air
u	exp. profile	4.7 10^{-3} kg/s	3.3 m/s
T	305 K	exp. profile	294 K
Y_k	CH_4:88%	exp. profile	O_2:23%
	H_2:12%		N_2:77%

Table 1: Inlet conditions on the three inlet boundaries of the domain.

Synthetic turbulence at the fuel inlet is generated by the Pamiès condition [6] and the Dynamic Smagorinsky model is applied. LES are performed using the variable density Low-Mach number solver of YALES2 [7].

Flame topology analysis

To assess the no-model assumption for TCI, a subgrid scale Damköhler number $Da_{sgs} = \tau_{sgs}/\tau_{chem}$ was computed, as proposed by [8]. $Da_{sgs} < 1$ means that the effect of the subgrid scales mixing on the chemistry modeling is insignificant. 9% of the cells located in the flame front are such as $Da_{sgs} > 1$. It would thus be interesting to perform a simulation using a TCI model.

The temperature and CO mass fraction numerical profiles are in good agreement with the experimental data in Fig. 3, near and far the fuel nozzle. The peaks

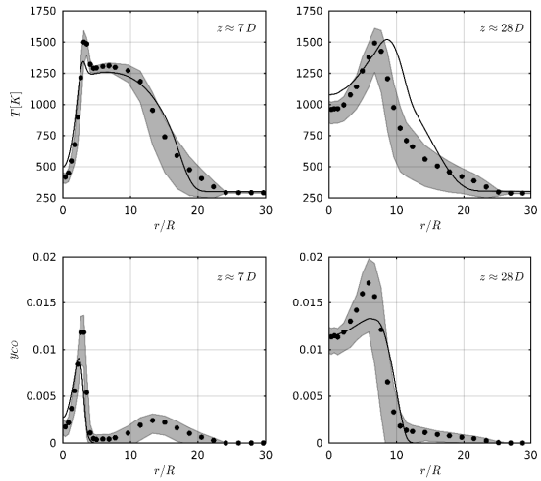

Figure 3: Mean temperature and CO mass fractions profiles, LES (–), Experimental (•).

are correctly located but the maximum values are underpredicted. This seems to be caused by a temperature level in the coflow also lower than in the measurements. Contrary to what one would expect, the predicted temperature peaks are not overestimated due to the assumption of neglecting TCI modeling.

The instantaneous heat release $\dot{\omega}_T$ and temperature T allows to observe that the species and temperature gradients are fairly resolved (Fig. 4). Their order of magnitude in the flame front, separating the fuel and the oxygen of the coflow, are close to those obtained with the 1D counterflow flame in Cantera.

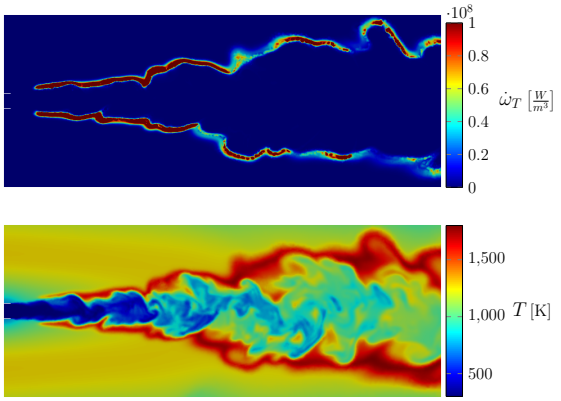

Figure 4: Mid-planes of instantaneous heat release and temperature.

Conclusion

The investigations carried out show that the TCI modeling can be neglected on the JHC burner using fine grids. However, given the distribution of Da_{sgs}, a simulation including a TCI-model, e.g. the Partially Stirred Reactor (PaSR) model, will be performed. This will allow to refine the conclusions about TCI modeling influence.

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