Large Eddy Simulation of diluted combustion

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1 Introduction

Recirculating burnt gases exist in most combustion systems where fuel and oxidizer are mixed with combustion products before they enter the main combustion zone. Those recirculating hot products carry thermal energy that may help to flame stabilization. They are also useful to dilute the reaction zones, which homogenizes the mixture and avoids the large temperature levels responsible for NOx emissions. So far, only few studies have discussed dilution by burnt gases in the context of turbulent combustion modeling [3]. In the present paper, Large-Eddy Simulation (LES) of such a combustion problem is addressed. LES of a methane-air jet turbulent flame developing in a vitiated coflow experiment reported by Cabra *et al* [1] are performed using fully detailed methane/air tabulated chemistry coupled with Sub-Grid Scale (SGS) presumed probability density functions.

2 LES of a turbulent diluted jet-flame

2.1 Conditions of the Cabra *et al.* experiment

The exact chemical composition and mass flow rate of recirculating burnt gases are often difficult to accurately calibrate and measure in real combustion chambers. To progress in the understanding of flame stabilization in environments where burnt gases dominate, Cabra *et al.* [1] have designed a laboratory burner in which the injection conditions of reactants and hot products are fully determined. In addition to detailed scalar measurements, Reynolds Average Navier Stokes Simulation (RANS) were also reported in Cabra *et al.* [1]. The burner consists of a round fuel jet issuing into a coflow of hot combustion products. This vitiated coflow is obtained from Hydrogen/Air lean premixed combustion (equivalence ratio $\phi = 0.4$) and it is mainly composed of H_2O and air flowing at 1350 K. The central fuel jet mixture is composed of 33% CH_4 and 67% air, by volume (equivalence ratio $\phi = 4.4$). The bulk velocity of the fuel jet and of the coflow velocity are of the order of 100 m/s and 5.4 m/s respectively. The geometry of the burner and the operating conditions are summarized in Table 1. This burner configuration was first used to study H_2/N_2 jet flame in vitiated coflow [2].

	Re	D (mm)	V (m/s)	T (K)	X_{O_2}	X_{N_2}	X_{H_2O}	X_{CH_4}
FUEL JET	28 000	4.57	100	320	0.15	0.52	0.0029	0.33
COFLOW	23 300	210	5.4	1 350	0.12	0.73	0.15	0.0003

Table 1: Conditions for the lifted methane-air jet flame in a vitiated coflow. Re: Reynolds number, D: Diameter, T: Temperature, X: Mole fraction, from Cabra *et al.* (2005).

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2.2 LES procedure

The SGS flame structure may be approximated using Presumed Conditional Moment (PCM), a closure based on Beta-shape presumed probability density function that was initially formulated in a RANS context [11], then extended to LES of premixed turbulent combustion [4]. Filtered scalars and sources may be cast in the form:

$$\widetilde{\varphi}(\underline{x},t) = \int_0^1 \left(\overline{\varphi|Z^*;\underline{x},t}\right) \widetilde{P}(Z^*;\underline{x},t)\, dZ^* \tag{1}$$

where Z is the mixture fraction.

In the flame under study, combustion is likely to start with autoignition, to be rapidly followed by flame propagation. But when autoignition cannot initially occur, flame propagation may be the stabilizing mechanism. The conditional filtered means $\left(\overline{\varphi|Z^*;\underline{x},t}\right)$ must be organized to capture this peculiar structure of the lifted flame in mixture fraction space. Accounting for those observations and for the fact that chemical tables are almost the same for low levels of the progress of the reaction, it is proposed to approximate $\left(\overline{\varphi|Z^*;\underline{x},t}\right)$ from the autoignition (AI) and premixed flamelet (PF) tables according to:

$$\left(\overline{\varphi|Z^*;\underline{x},t}\right) = (1-\overline{c}) \int_0^1 \varphi^{AI}(Z^*,c^*)\overline{P}(c^*;\underline{x},t)dc^* + \overline{c} \int_0^1 \varphi^{PF}(Z^*,c^*)\overline{P}(c^*;\underline{x},t)dc^* \tag{2}$$

where $c = Y_c/Y_c^{Eq}$ is a progress variable. $\varphi^{AI}(Z^*,c^*)$ is obtained by solving auto-ignition problems for all attainable fresh-gas compositions upstream of the turbulent flame base and by tabulating them using the FPI technique [6]. Similarly, $\varphi^{PF}(Z^*,c^*)$ derives from the tabulation of freely propagating laminar premixed flamelets, both tables have been derived using the GRI 3.0 methane-air mechanism [7]. Mixture fraction and progress variable are assumed statistically independent (notice that this applies to c that is a normalized quantity, but not to the progress of reaction Y_c or to any other quantity $\varphi = Y_i$ of the tables). Then, $\overline{c} = \overline{\rho Y}_c/\overline{\rho Y}_c^{Eq}$ and $c_v = Y_{c_v}/\widetilde{Y_c^{Eq^2}} + \widetilde{Y}_c^{\,2}(1/\widetilde{Y_c^{Eq^2}} - 1/\widetilde{Y_c^{Eq}}^{\,2})$, where $c_v = \widetilde{cc} - \tilde{c}\,\tilde{c}$ and $Y_{cv} = \widetilde{Y_cY_c} - \widetilde{Y}_c\,\widetilde{Y}_c$ denote SGS variances.

The quantities necessary to presume the PDFs, $\widetilde{Z}$, Z_v, $\widetilde{Y}_c$ and $\widetilde{Y_cY_c}$ are obtained from their balance equations:

$$\frac{\partial \overline{\rho}\widetilde{Z}}{\partial t} + \nabla\cdot\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Z} = -\nabla\cdot\overline{\tau}_Z + \nabla\cdot\left(\overline{\rho}\mathcal{D}\nabla\widetilde{Z}\right) \tag{3}$$

$$\frac{\partial \overline{\rho}Z_v}{\partial t} + \nabla\cdot\overline{\rho}\widetilde{\mathbf{u}}Z_v = -\nabla\cdot\overline{\tau}_{Z_v} + \nabla\cdot\left(\overline{\rho}\mathcal{D}\,\nabla\widetilde{Z}_v\right) - 2\overline{\tau}_{Z_v}\cdot\nabla\widetilde{Z} - 2\overline{s}_{\chi_Z} \tag{4}$$

$$\frac{\partial \overline{\rho}\widetilde{Y}_c}{\partial t} + \nabla\cdot\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y}_c = -\nabla\cdot\overline{\tau}_{Y_c} + \nabla\cdot\left(\overline{\rho}\mathcal{D}\,\nabla\widetilde{Y}_c\right) + \overline{\rho}\widetilde{\dot{\omega}}_{Y_c} \tag{5}$$

$$\frac{\partial \overline{\rho}\widetilde{Y_cY_c}}{\partial t} + \nabla\cdot\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Y_cY_c} = -\nabla\cdot\overline{\tau}_{Y_cY_c} + \nabla\cdot\left(\overline{\rho}\mathcal{D}\nabla\widetilde{Y_cY_c}\right) - 2\overline{\rho}\overline{S}_{\chi_{Y_c}} - 2\overline{\rho}D|\nabla\widetilde{Y}_c|^2 + 2\overline{\rho}\widetilde{Y_c\dot{\omega}_{Y_c}} \tag{6}$$

The SGS turbulent fluxes, $\overline{\tau}_Z$, $\overline{\tau}_{Z_v}$, $\overline{\tau}_{Y_c}$ and $\overline{\tau}_{Y_cY_c}$ are expressed using the filtered structure function closure of Lesieur *et al* (2005) [9]. The SGS scalar dissipation rates are modeled as $\overline{s}_{\chi_Z} = \overline{\rho}Z_v/(\Delta^2\nu_T)$ and $\overline{s}_{\chi_{Y_c}} = \overline{\rho}Y_{cv}/(\Delta^2\nu_T)$ where Δ is the characteristic filter size and ν_T the SGS eddy viscosity given by filtered structure function modeling. The filtered sources of progress of reaction $\widetilde{\dot{\omega}}_{Y_c}$, $\widetilde{Y_c\dot{\omega}_{Y_c}}$ and of energy are expressed from the relations 1 and 2.

The set of Navier-Stokes equations in their fully compressible form are solved together with above equations. A fourth-order finite volume skew-symmetric-like scheme proposed by Ducros *et al.* [5] is adopted for the spatial derivatives. This scheme was specifically developed for LES and it is here combined with second-order Runge Kutta explicit time stepping. Acoustic waves are included in the fully compressible formulation and Navier-Stokes characteristic boundary conditions are retained [10]. The mesh is composed of 2150,000 nodes with a characteristic mesh size h that verifies 0.3 mm $< h <$ 2.5 mm. Its spanwise and streamwise lengths are 20D and 90D respectively. Turbulence is generated in the inlet plane following the procedure proposed by Klein *et al* [8].

2.3 LES results

The jet centerline average, $<\widetilde{T}>$ computed from the filtered temperature , and fluctuations, $<\widetilde{T}\widetilde{T}> - <\widetilde{T}><\widetilde{T}>$, are presented figure 1-right. The good agreement with experiment indicates that the position of the lifted turbulent flame base is well captured. The radial profile of the average temperature (fig. 1-left) shows also a fairly good agreement with the experimental measurement. Those quantities have been averaged over 4 flow times (measured from average inlet velocity and streamwise length of the computational domain). Radial profiles of mean temperature are also averaged in space using the axi-symmetric character of the flow. The axial evolutions of the Favre averaged mass fraction of species, H_2O, CO_2, O_2, CO, NO and OH, are plotted in figure 2. These results suggest that chemistry tabulation and the SGS LES modeling contribute to provide reliable information on species concentrations.

The capability of the modeling closure to reproduce the sensitivity of the lift-off height to changes in the co-flow velocity and temperature will be investigated and compare towards experiment.

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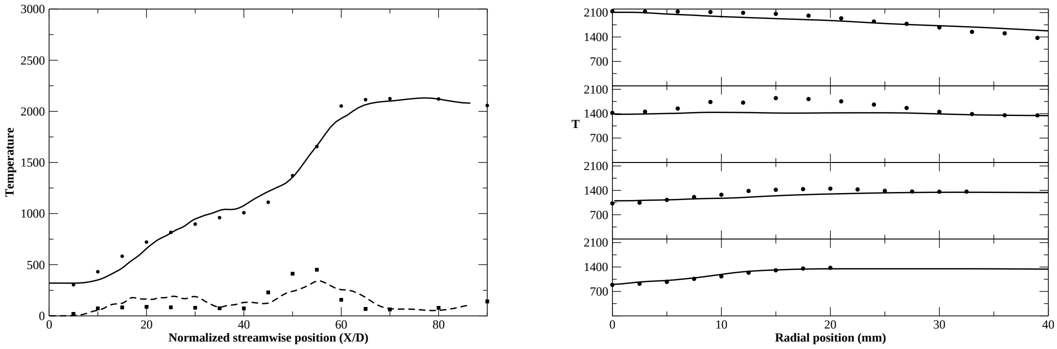

Figure 1: Left: Axial profile of Favre averaged (line and circle) and RMS (dash line and square) temperature on the centerline of the jet. Right : Radial profiles of Favre averaged temperature From bottom to top, streamwise position X/D = 30, 40, 50, 70. Symbols: Measurements. Line: LES.

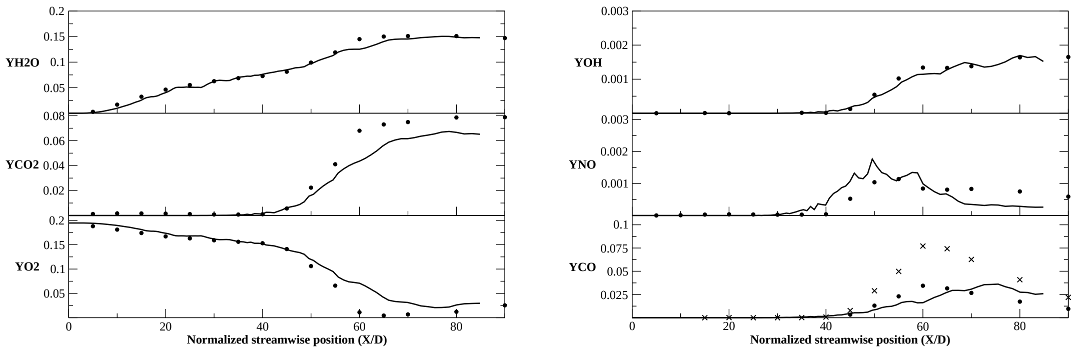

Figure 2: Axial profiles of Favre averaged mass fractions (O_2, CO_2, H_2O, CO, NO and OH). Symbols: Measurements. Line: LES. For Y_{CO} : circles represent Raman measurements and crosses LIF measurements.

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