Large Eddy Simulation of lifted turbulent jet diffusion flames

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1 Introduction

Partial premixing is observed in nonpremixed flames when fuel and oxidizer have mixed without burning. This may result from frozen flow mixing found before ignition or from local quenching. In most devices where a spray of liquid fuel is injected, partially premixed flame propagation is observed, as in a gasoline direct injection engine or also in aircraft engines. Therefore in the modeling of many combustion systems, partially premixed combustion should be accounted for [1, 2].

Lifted turbulent jet flame is a laboratory simplified situation where partially premixed combustion is expected. At the flame base, combustion starts in a mixture composed of fuel and oxidizer that have been partially mixed. Downstream of this turbulent flame base, a turbulent diffusion flame develops. Various experimental and numerical studies have concluded that triple flamelets and edge-flames are the basic ingredients of the turbulent flame base [3].

The modeling of these lifted flames requires the simultaneous description of the trailing diffusion flame and of locally propagating partially premixed flames defined for a distribution of equivalence ratios. A procedure based on the topology of the species field was recently proposed to distinguish in simulations between premixed and diffusion combustion [4]. Combining this approach with Large Eddy Simulation (LES) for the premixed and non-premixed regimes, a subgrid combustion closure for partially premixed flame has been proposed [5]. In the following, lifted turbulent methane air flames are simulated using this formalism. The statistical properties of the flame base are collected in the LES, they compare well with experimental observations in term of flow velocity and reveal some properties of partially premixed turbulent combustion.

2 Partially premixed flamelets in LES

For LES of nonpremixed turbulent flames, where partial premixing is expected, it was recently proposed [5] to decompose the large eddy mass fractions fields $\widetilde{Y}_i$ into $\widetilde{Y}_{i,p}$, a premixed part, and, $\widetilde{Y}_{i,d}$, a nonpremixed part:

$$\widetilde{Y}_i = \xi_p \widetilde{Y}_{i,p} + (1 - \xi_p) \widetilde{Y}_{i,d} \tag{1}$$

where $\widetilde{Y}_{i,p}$ and $\widetilde{Y}_{i,d}$ are calculated from: a progress variable c for premixed combustion ($c = 0$ in fresh gases and $c = 1$ in fully burnt products), and a mixture fraction Z for nonpremixed flames (Z is a passive scalar with $Z = 0$ in oxidizer and $Z = 1$ in the fuel stream). In the subgrid combustion model these quantities are simultaneously resolved at the LES filtered level.

In Eq. 1, ξ_p is an indicator of local premixing, it is approximated from the resolved large eddy field:

$$\xi_p = \frac{1}{2}\left(\frac{\nabla\widetilde{Y}_F\cdot\nabla\widetilde{Y}_O}{|\nabla\widetilde{Y}_F||\nabla\widetilde{Y}_O|}+1\right) \tag{2}$$

$\xi_p = 1$ corresponds to fully premixed reactants at the molecular level and $\xi_p = 0$ to diffusion flames [4]. The filtered species gradients entering ξ_p define the main flame topology and the same combustion regime is expected at both resolved and subgrid levels.

The premixed flame featuring a non-uniform equivalence ratio is captured extending the subgrid combustion closure of Veynante and coworkers [6]. A transport equation for the mass filtered progress variable $\widetilde{c}$ is derived, unknown terms are closed leading to:

$$\frac{\partial\overline{\rho}\widetilde{c}}{\partial t}+\nabla\cdot(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{c}) = \nabla\cdot\left[\left(\overline{\rho}_u\frac{\widetilde{S}_L\Delta}{16\sqrt{6/\pi}}+\frac{\mu_t}{\sigma_t}\right)\nabla\widetilde{c}\right]+4\overline{\rho}_u\widetilde{S}_L\Xi\sqrt{\frac{6}{\pi}}\frac{\widetilde{c}(1-\widetilde{c})}{\Delta} \tag{3}$$

where μ_t is the subgrid turbulent viscosity, σ_t is a turbulent Schmidt number and Δ a LES filter size. The wrinkling factor Ξ is assumed constant ($\Xi = 1.1$). In nonpremixed flames, to account for partially premixed flamelets, we compute the mean density of fresh gases $\overline{\rho}_u$ and the burning velocity $\widetilde{S}_L$ from the knowledge of $\rho_u(Z)$ and $S_L(Z)$, the response of these quantities to a non-uniform composition of fresh gases determined using the GRI methane - air chemical kinetics. $S_L(Z)$ is averaged using the mixture fraction pdf $\widetilde{P}(Z^*)$:

$$\widetilde{S}_L = \int_0^1 S_L(Z^*)\widetilde{P}(Z^*)\,dZ^* \tag{4}$$

The closed transport equation for the filtered mixture fraction is written:

$$\frac{\partial\overline{\rho}\widetilde{Z}}{\partial t}+\nabla\cdot(\overline{\rho}\widetilde{\mathbf{u}}\widetilde{Z}) = \nabla\cdot\left[\left(D+\frac{\mu_t}{\sigma_t}\right)\nabla\widetilde{Z}\right] \tag{5}$$

a scale similarity hypothesis [7] is chosen to estimate $\widetilde{(\widetilde{Z}-Z)^2}$, the mixture fraction fluctuations at the subgrid level. $\widetilde{Z}$ and $\widetilde{(\widetilde{Z}-Z)^2}$ are then retained to parameterize the beta mixture fraction pdf $\widetilde{P}(Z^*)$. A basic flamelet model is utilized for the diffusion flame part giving $\widetilde{Y}_{i,d}$.

The links between the premixed and nonpremixed parts are evidenced assuming thin partially premixed flame fronts, in a BML context [8] one may write [5]:

$$\widetilde{Y}_{F,p} = (1-\overline{c})\,Y_{F,o}\widetilde{Z}+\overline{c}\,\widetilde{Y}_F^{Eq} \tag{6}$$

$$\widetilde{Y}_{O,p} = (1-\overline{c})\,Y_{O,o}(1-\widetilde{Z})+\overline{c}\,\widetilde{Y}_O^{Eq} \tag{7}$$

$\overline{c}$ is estimated from $\widetilde{c}$ using the basic BML relation, $\overline{c} = \overline{\rho}_u\widetilde{c}/(\overline{\rho}_b+(\overline{\rho}_u-\overline{\rho}_b)\widetilde{c})$, where the subscripts $_u$ and $_b$ denote fresh and burnt gases respectively.

The Lagrangian dynamic model of Meneveau et al. [9] is retained to calculate μ_T and σ_T. The fourth order finite volume skew-symmetric-like scheme of Ducros et al. [10] is chosen for spatial discretization, combined with a second order Runge Kutta time stepping. To save a great amount of cpu time, the flow is first analyzed using two-dimensional simulations.

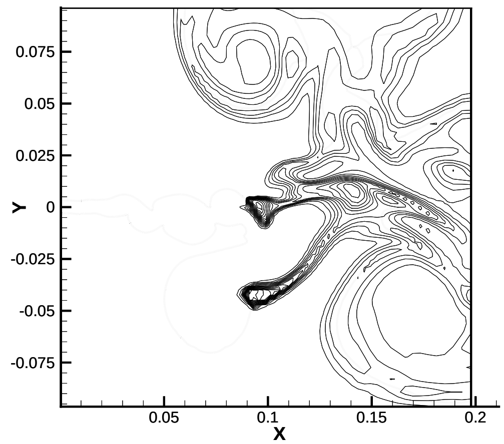

Figure 1: Iso-contour of temperature at the flame base, Line: Stoichiometric mixture. Lengths are in meter.

3 LES of methane - air turbulent lifted flames

The lifted flame configuration is the one studied experimentally by Muniz and Mungal [11]. A round methane jet of diameter $d_o = 4.8\,mm$ is surrounded by an air coflow. The inlet velocities are $U_{CH_4} = 14\,m.s^{-1}$ and $U_{Air} = 0.27\,m.s^{-1}$, corresponding to case III of [11]. The flame is lifted and combustion starts in a partially premixed regime at a mean streamwise position located at $14\,d_o$. In the simulations the grid is 128X128 clustered near the burner exit. Only the flame base is simulated, the length of the square computational domain is $41\,d_o$.

Figure. 1 shows the iso-stoichiometric line and the temperature field. Unsteady mixing resulting from the roll-up of the shear layers is visible. The unsteady simulations reveal that the dynamics of stabilization regions depends on the continuous interaction between extremities of reaction zones and turbulence (Fig. 1). When

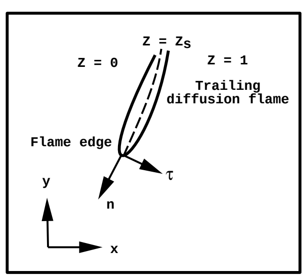

Figure 2: Sketch of the local coordinates attached to a reaction zone extremity.

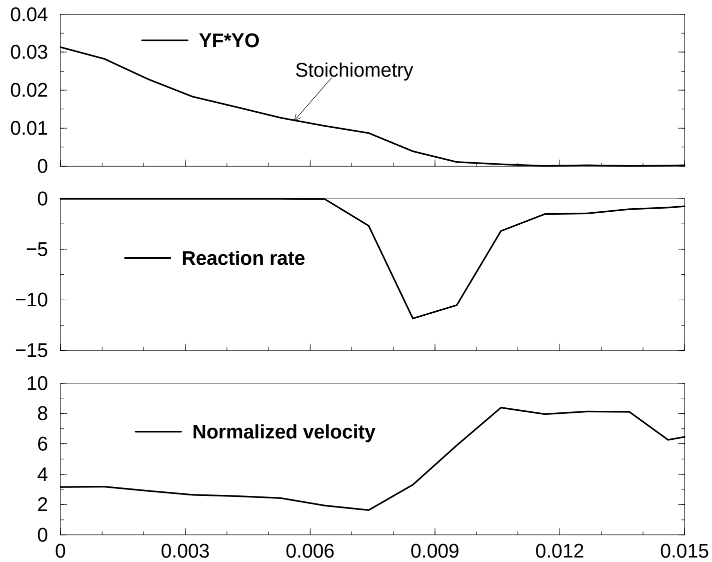

Figure 3: Along the stoichiometric line of a reaction zone extremity. Top: $\widetilde{\phi} = \widetilde{Y}_F \widetilde{Y}_O$. Middle: Filtered reaction rate. Bottom: Flow velocity.

studying the topology of the flame base in their experiments, Muniz and Mungal found that velocity profiles taken across the flame base feature properties similar to those observed in triple flames. Suggesting that the reaction zone extremities have strong similarities with triple flames and edge flames [2, 4].

In order to focus on the possible role of those reaction zone extremities found at the flame base in LES, quantities are plotted using a local coordinate system (Fig. 2) attached to one representative reaction zone extremity observed along the partially premixed front. Values are collected along the direction $\mathbf{n}$ as defined in Fig. 2, thus following the stoichiometric line.

The filtered partially premixed fraction $\widetilde{\phi} = \widetilde{Y}_F \, \widetilde{Y}_O$ indicates that premixing has developed upstream of the local edge flame where $\xi_p \approx 1$ (Fig. 3-top). Then, the local premixed front consumes the reactants for the stoichiometric value $\widetilde{\phi}_s = Y_{F,o} Y_{O,o} Z_s (1 - Z_s)$, this is visible from $\widetilde{\phi}$ and the burning rate (Fig. 3-top and middle). The velocity profile following the stoichiometric line of a turbulent edge flame as captured by LES is shown in Fig. 3-bottom. The velocity is normalized by S_L^o, the stoichiometric burning velocity of a premixed flame. The complex tribrachial structure of the triple flame cannot be resolved by LES, however in both LES and measurements, the velocity profile features strong similarities with those observed in triple flames [11], with an upstream velocity of the order of three times S_L^o. In other words, in the experiment and in the LES, the collection of reaction zone extremities (or edge flames) stabilizing the lifted flame, continuously follow within the turbulent mixture, the zone of low velocity that is of the order of a triple flame speed.

4 Conclusion and perspectives

A novel subgrid turbulent combustion model is discussed and tested for LES of partially premixed flames. The simulation of a lifted turbulent jet flame compares well with experiments in term of the major flame base properties. The simulation confirms that local triple flames and edge flames plays a dominant role in such lifted flames.

The subgrid combustion model providing encouraging results for two-dimensional simulations, three-dimensional simulation are now carried out to carefully study the dynamics of the three-dimensional flame base.

References

[1] N. Peters. *Turbulent Combustion*. Cambridge University Press, 2000.

[2] L. Vervisch. Using numerics to help understand nonpremixed turbulent flames. In *Twenty-Eighth Int. Symposium on combustion*, pages 11–24, 2000.

[3] K. A. Watson, K. M. Lyons, J. M. Donbar, and C. D. Carter. Observations on the leading edge in lifted flame stabilization. *Combust. and Flame*, 119(1/2):199–202, 1999.

[4] V. Favier and L. Vervisch. Edge flames and partially premixed combustion in diffusion flame quenching. *Combust. Flame*, Accepted, to appear.

[5] Pascale Domingo, Luc Vervisch, and Ken Bray. Accounting for partially premixed flamelets in les of non-premixed turbulent combustion. *Submitted*, 2001.

[6] M. Boger and D. Veynante. Large eddy simulation of a turbulent premixed v-shaped flame. In C. Dopazo, editor, *Advances in Turbulence*, pages 449 – 452. CIMNE, BARCELONA, isbn: 84-89925-65-8 edition, 2000.

[7] A. W. Cook and J. J. Riley. A subgrid model for equilibrium chemistry in turbulent flows. *Phys. Fluids*, 8(6):2868–2870, 1994.

[8] K.N.C. Bray and P. A. Libby. Recent developments in the bml model of premixed turbulent combustion. In P.A. Libby and F.A. Williams, editors, *Turbulent Reacting Flows*, pages 116–151. Academic Press London, 1994.

[9] C. Meneveau, T. S. Lund, and W. Cabot. A lagrangian dynamic subgrid-scale model of turbulence. *J. Fluid Mech.*, pages 353–386, 1996.

[10] F. Ducros, F. Laporte, T. Soulères, V. Guinot, P Moinat, and B. Caruelle. High-order fluxes for conservative skew-symmetric-like schemes in structured meshes: application to compressible flows. *J. Comput. Phys.*, 161:114–139, 2000.

[11] L. Muñiz and M. G. Mungal. Instantaneous flame-stabilization velocities in lifted-jet diffusion flames. *Combust. Flame*, 111(1/2):16–31, 1997.