Dynamically thickened flame LES model for premixed and non-premixed turbulent combustion

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A new LES subgrid scale turbulent combustion model, adapted to combustion regimes which are neither perfectly premixed nor non-premixed, is tested in a simplified configuration. This model does not require any *a priori* assumption on the flame structure and is able to compute flows where both premixed and non-premixed flamelets coexist. Three combustion regimes identified in an experiment conducted at Ecole Centrale Paris, anchored, lifted and blown-off flames, are successfully recovered in numerical simulations.

1. Motivations and objectives

Turbulent flames in most gas turbines are neither perfectly premixed nor perfectly non-premixed and require the development of large eddy simulation (LES) model adapted to this situation. Unfortunately, very few studies have tried to address these problems because they gather the complexities of pure mixing (without combustion) of ignition, of partially or perfectly premixed combustion, and of non-premixed combustion. All of these regimes may be encountered simultaneously in a gas turbine, and a proper model should be able to handle all of them. This is especially true for recent technologies like LPP (lean premixed prevaporized) combustors which are designed to mainly operate in a lean premixed mode but are prone to flame flashback (i.e. a flame propagation upstream of its designed location), a regime dominated by diffusion flames. Being able to predict flashback requires models which are not yet available.

Many LES studies have been published for mixing (Pierce & Moin (1998)), for premixed flames (Bourlioux Moser & Klein (1996), Veynante & Poinsot (1997), Im, Lund & Ferziger (1997), Piana, Ducros & Veynante (1997), Boger *et al.* (1998), Colin *et al.* (2000a)), or for diffusion flames (Desjardins & Frankel (1999), Moin, Pierce & Pitsch (2000)). But all of these models are derived taking explicitly into account the flame topology, premixed or not, thereby limiting the predictive character of simulations when the exact regime of combustion is not *a priori* known.

In the present work, a new model called DTF (Dynamic Thickened Flame) is proposed to compute mixing, diffusion, and premixed flames simultaneously. This objective is achieved modifying the thickened flame model derived for premixed flames. Instead of using a constant thickening factor (Colin *et al.* (2000a)), a local thickening factor F is active only in the vicinity of the flame front ($F > 1$) and relaxes to $F = 1$ (no effect) far away from the flame. A potential advantage of the model is that outside of the flame zones, thickening is suppressed and mixing can be predicted correctly. This point

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is important in gas turbines where pure mixing (without chemical reaction), premixed, and non-premixed zones may coexist.

The DTF model (Section 2), is tested in a two-dimensional geometry corresponding to an experimental burner developed at Ecole Centrale Paris and described in Section 3. Simple one-dimensional tests are presented in Section 4. Section 5 presents LES runs and discusses numerical results.

All computations are performed with AVBP, the LES code developed by CERFACS. The numerical scheme is third order both in space and time (Colin & Rudgyard (2000b)).

2. Principle of the Dynamically Thickened Flame (DTF) model

In this work, a simple one-step scheme is used to describe propane/air chemistry:

$$C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow 3CO_2 + 4H_2O + 18.8N_2 \tag{2.1}$$

The fuel consumption rate is given by:

$$\dot{\omega}_F = A\nu_F W_F \left(\frac{\rho Y_F}{W_F}\right)^{\nu_F} \left(\frac{\rho Y_O}{W_O}\right)^{\nu_O} \exp\left(-\frac{T_a}{T}\right) \tag{2.2}$$

where T_a is the activation temperature, W_F and W_O are respectively the atomic weights of propane ($W_F = 44$) and oxygen ($W_O = 32$). The prexponential constant A is fitted to provide correct flame speeds for lean premixed flames when compared to full chemistry results. Chemical parameters are:

$$A = 1.65.10^{11}\,\mathrm{cgs} \quad ; \quad T_a = 15080\,\mathrm{K} \quad ; \quad \nu_F = 0.5 \quad ; \quad \nu_O = 1 \tag{2.3}$$

The fuel mass fraction Y_F balance equation is:

$$\frac{\partial \rho Y_F}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \nabla \cdot (\rho \mathcal{D} \nabla Y_F) - \dot{\omega}_F \tag{2.4}$$

where usual notations are retained.

The thickened flame model is an extension of the initial model proposed by Butler & O' Rourke (1977) for premixed flames. These authors showed that multiplying species and heat diffusion coefficients by a factor F (i.e. $\mathcal{D}$ becomes $\mathcal{D}F$) and decreasing the exponential constant by the same factor F (A is replaced by A/F) in Eq. (2.4) provides a flame propagating at the same laminar flame speed s_l^0 than the non-thickened flame but its thickness is increased by a factor F and becomes $\delta_L^1 = F\delta_L^0$. Adjusting F to sufficiently large values (typically between 10 and 100 in most gas turbines) allows the flame to be resolved on an LES grid.

This initial model can be easily extended to dynamic thickening, depending on time and spatial location, by recognizing that a premixed flame where the thickening factor F changes spatially still propagates at the laminar flame speed s_l^0 (Cuenot, 2000, private communication). The mathematical proof of this finding is formally similar to the derivation of the Howarth-Dorodnitzyn transformation introduced to analyze variable density flows under boundary layer approximations as constant density flows (Williams (1985)). The thickening factor F may then be modulated from large values inside the reaction zone (where the reaction rate, inducing large gradients, has to be numerically resolved) to unity away from the flame front (to avoid a modification of mixing description by changing molecular diffusion coefficients), keeping the right propagation speed of a laminar premixed flame. The sensor used to determine whether the flame should be

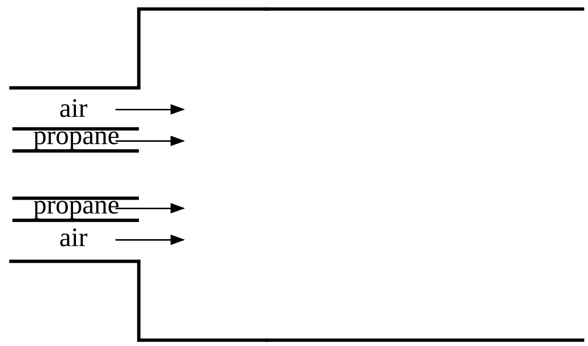

FIGURE 1. Dump-stabilized burner configuration. Experiment developed at EM2C lab., Ecole Centrale Paris, France.

thickened or not is based on a "Arrhenius-like" expression:

$$\Omega = Y_F^{\nu_F} Y_O^{\nu_O} \exp\left(-\Gamma \frac{T_a}{T}\right) \tag{2.5}$$

This sensor detects the presence of the reaction zone but is active in a broader zone than the reaction rate because of the Γ parameter which artificially decreases the activation temperature ($\Gamma < 1$). The sensor Ω controls the value of the thickening coefficient F through:

$$F = 1 + (F_{max} - 1) \tanh\left(\beta \frac{\Omega}{\Omega_{max}}\right) \tag{2.6}$$

where Ω_{max} is the maximum of Ω (which can be determined analytically for a stoichiometric premixed flame) and β is a parameter controlling the thickness of the transition layer between thickened and non-thickened zones.

As shown by Angelberger *et al.* (1998), the thickening procedure allows propagation of the flame on a coarse grid but reduces the flame response to the smallest turbulent motions. To overcome this difficulty, Angelberger *et al.* (1998) and Colin *et al.* (2000a) have derived an efficiency function E to account for the unresolved flame wrinkling. This function E depends on the thickening factor F, the length scale Δ_e/δ_L^0, and the velocity u'_{Δ_e}/s_L^0 ratios (Δ_e is the combustion LES filter size and u'_{Δ_e} the subgrid scale rms velocity) and is used, as a first step, without modification in the present work. In the practical implementation of the thickened flame model, the molecular diffusion coefficient $\mathcal{D}$ is replaced by $EF\mathcal{D}$ and the pre-exponential constant A of the Arrhenius law (Eq. 2.2) by EA/F.

3. Experimental configuration and stability maps

Fig. 1 presents the experimental configuration developed at the EM2C laboratory (Ecole Centrale Paris, France) and used here to test the DTF model. Two propane streams are injected through small slots (5 mm height) into an air coflow. Two backward facing steps (25 mm height each) promote the flame stabilization. The combustion chamber, downstream of the fuel injector lips, is 300 mm long, 100 mm height, and 80 mm depth. The experiment is designed to produce two-dimensional flows to simplify optical diagnostics (CH and C_2 radical emission, laser induced fluorescence on OH radical,...) and model developments and validations. The maximum burner power is 300 kW.

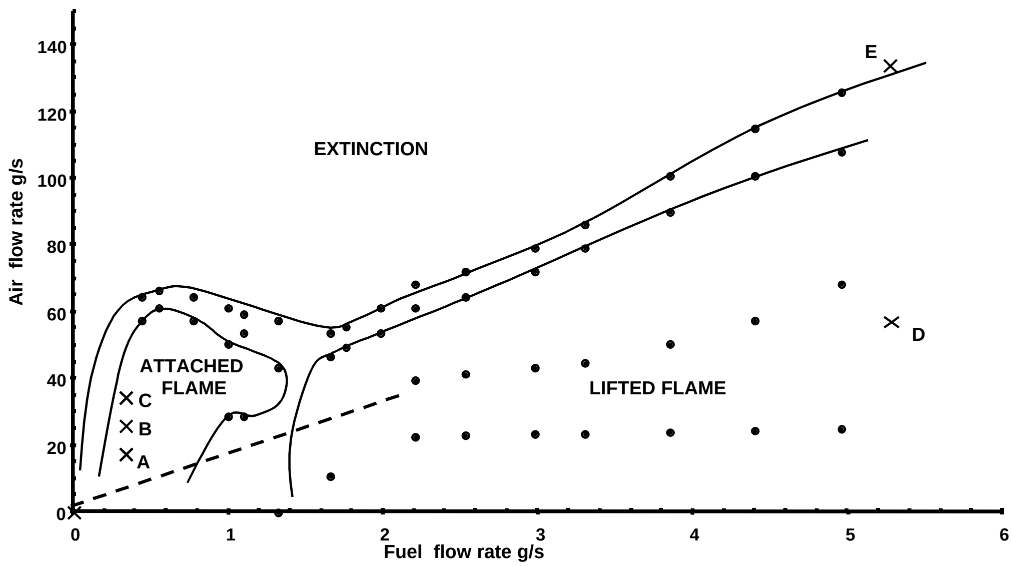

Figure 2. Combustion regimes observed in the EM2C burner displayed in Fig. 1 and plotted as a function of the fuel and air mass flow rates. The global stoichiometric line, where fuel and air are injected in stoichiometric proportions, is also indicated.

The burner exhibits various operating regimes, summarized in terms of air and fuel mass flow rates in Fig. 2:

• *Rim stabilized (anchored) flames*: for low fuel and air flow rates powers and, accordingly, low burner powers, flames are stabilized a few millimeters downstream of the fuel injectors (Fig. 3a). This regime corresponds to "anchored" flames.

• *lifted flames*. For higher reactant flow rates (higher powers) and rich overall equivalence ratio (excess of fuel compared to the among of air injected), the flames lift from the injectors and are stabilized a few cm downstream of the injectors in the vicinity of recirculation zones induced by the backward facing steps (Fig. 3b). This regime is referred here as "lifted" (flames are far from the injectors lips) but is very different from the so-called lifted flames encountered in jet diffusion flames without recirculation zones. Here, combustion is stabilized by the hot gases recirculating behind the steps near the injectors.

• *Extinction*. For high reactant flow rates but too lean overall equivalence ratio, the flame gets quenched.

• The transition from one regime to another is accompanied by oscillations (instabilities).

This simplified burner exhibits many characteristics observed in modern gas turbine burners: the existence of multiple flame regimes (anchored or lifted) and of sudden extinctions. This combustor appears, therefore, to be a good test configuration for models.

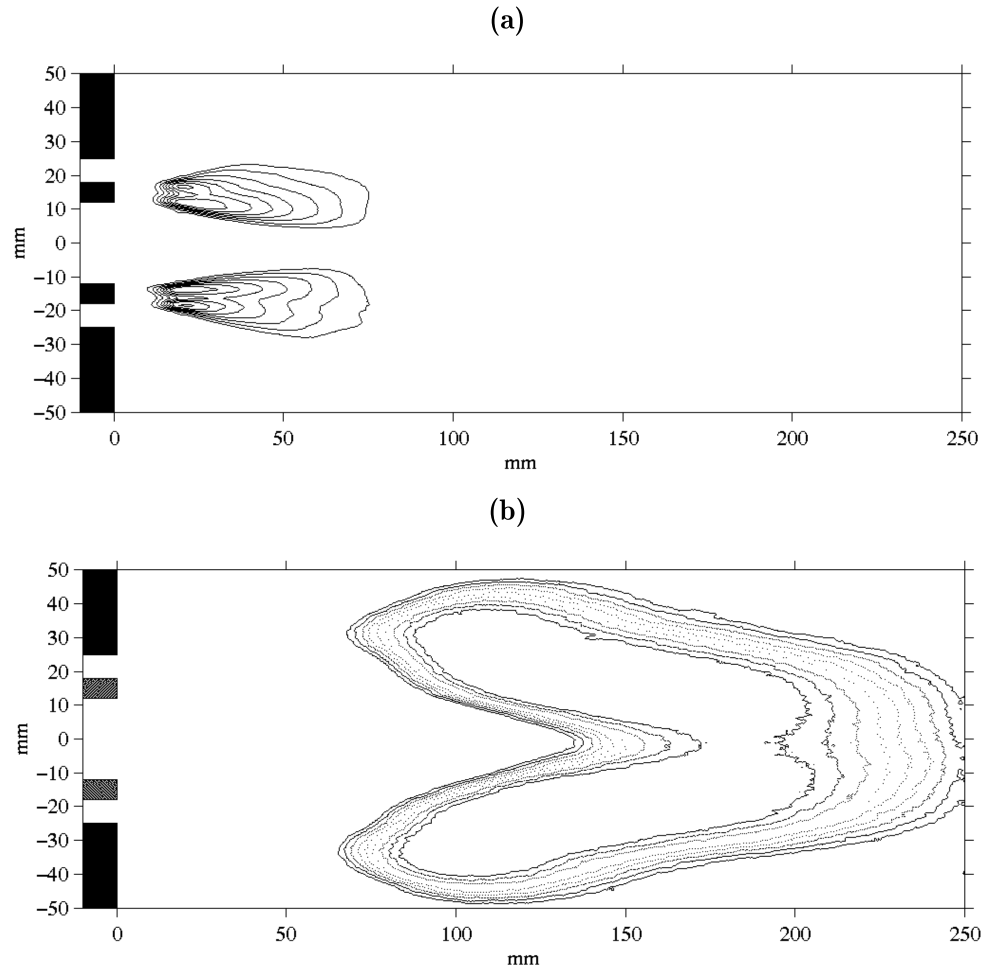

FIGURE 3. Combustion regimes observed in the EM2C burner and visualized using mean CH radical spontaneous emission, corresponding to the mean reaction rate. (a): "anchored flame" regime. The flame is stabilized in the vicinity on the fuel injectors but is not anchored on the lips. (b) "lifted flame" regime where the flame is stabilized by recirculation zones induced by the two backward facing steps. Experiments performed by B. Varoquié, EM2C Lab., Ecole Centrale Paris.

4. One-dimensional laminar premixed flame computations

As a first validation example, one-dimensional laminar premixed flames temperature profiles are compared in Fig. 4 for a non-thickened flame ($F = 1$), a thickened flame with constant thickening factor ($F = 20$ everywhere), and a dynamically thickened flame with $F_{max} = 20$.

For the chosen conditions ($P = 1$ atm, equivalence ratio $\phi = 0.6$, and fresh gases temperature $T_u = 300$ K), all flames propagate at the same speed $s_L^0 = 14$ cm/s. The thickened flames are obviously much broader and can be resolved with coarser grid meshes: the thermal thickness of the unthickened flame is 0.65 mm and becomes 13 mm for the two thickened flames. The dynamically thickened flame is slightly thinner than the initial

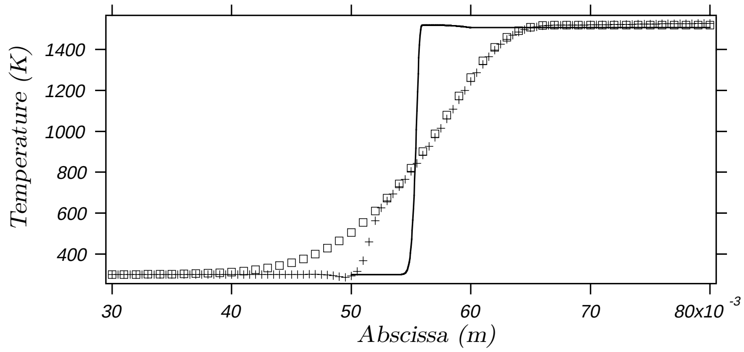

FIGURE 4. Temperature profiles for a non-thickened lean premixed propane/air flame (solid line), a thickened flame with F=20 (squares) and a dynamically thickened flame with $F_{max} = 20$ (crosses). Atmospheric pressure ($P = 1$ atm), fresh gases temperature $T_u = 300$ K, equivalence ratio $\phi = 0.6$.

Case	Fuel flow rate (g/s)	Air flow rate (g/s)	Global equivalence ratio ϕ	Air speed (m/s)	Fuel speed (m/s)	Reynolds number
Anchored (C)	0.33	35	0.15	13	0.6	23000
Lifted (D)	5	58	1.34	23	11	35000
Blow-off (E)	5	145	0.54	55	11	88000

TABLE 1. Operating flow conditions for LES tests. The Reynolds number is evaluated in the outlet section of the burner. The air and fuel speeds correspond to the maximum velocities measured in the air and fuel inlets. The global equivalence ratio ϕ compares the overall amount of fuel and air injected in the burner but is not the local equivalence ratio involved in laminar diffusion flames. Points C, D, and E are also displayed in Fig. 2.

thickened flame in the preheating zone because the sensor Ω is based on a reaction rate type formulation, but differences remain small.

5. LES results

LES were conducted for three regimes, referred to as B, D, and E (see Fig. 2). The first case, (C), corresponds to an anchored flame; in the second one, (D), the flame is lifted whereas a flame blow-off is expected in regime (E). Unresolved fluxes are modeled using a filtered Smagorinsky model (Nicoud & Ducros (1997)), and combustion is described using the DTF model (section 2). Two meshes were used: a coarse grid (62644 nodes) and a fine one (262000 nodes). For these first tests, two-dimensional simulations are performed and only the upper half of the burner is computed (the flow field is assumed to be symmetrical along the burner axis). All model parameters were kept constant for all simulations. Operating flow conditions are summarized in Table 1.

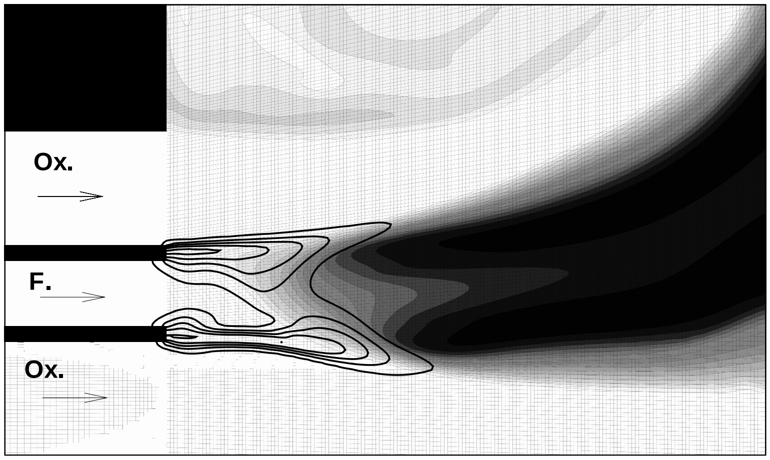

FIGURE 5. Anchored flame (case C): mixing index $Y_F Y_O$ (lines) and temperature (gray-scale) fields. Zoom in the vicinity of the upper fuel injector.

5.1. *Anchored flame (Case C)*

For low reactant flow rates and low powers, flames are stabilized in the vicinity of the fuel injector, but they do not touch the injector. A small lift-off height is observed experimentally (Fig. 3a) as well as in the LES results. Fig. 5 presents a view of the flow close to the fuel injector for case C: the mixing index $Y_F Y_O$ (lines) and the temperature (gray scale) fields are displayed.

The flame is stabilized by a couple of “triple flames”: one for the upper air jet and some part of the fuel stream, and another one for the central air jet and the rest of the fuel stream. Even though the attachment region flaps slightly, the structure of the zone close to the injectors appears rather steady. Downstream, pockets of burnt gases oscillate in the duct, but the anchoring mechanism seems unaffected by these flow perturbations. The recirculation zone does not contain hot gases and is not involved in the stabilization process.

5.2. *Lifted flame (Case D)*

For larger reactants flow rates and higher burner powers, the flame cannot remain attached to the injector lips and is stabilized by the recirculation zones. A typical snapshot of the flowfield in case D is presented in Fig. 6: the fuel mass fraction Y_F (gray scale) is superimposed on the reaction rate field and the two stoichiometric lines (bold lines). The first striking feature of this computation is that, even though fuel and oxidizer are injected separately into the burner, only a few flame zones exhibit a diffusion-like structure and lie around the stoichiometric iso-surface; in fact, strong mixing occurs before any combustion starts. When combustion begins, a strong premixed flame is observed. This premixed flame burns rich mixtures and leaves fuel in its product. This fuel can burn with air downstream or in the recirculation zone.

This description is confirmed by cuts performed at two locations (A and B). For location A on Fig. 6, a cut (Fig. 7a) reveals a typical diffusion flame structure where oxidizer and fuel are found on separate sides of the flame front. However, the fuel found at point A is mixed with burnt products so that the diffusion flame structure observed for this point is very different from the usual fuel (cold)/oxidizer configuration used in flamelet models. First, the maximum fuel mass fraction is about $Y_F \approx 0.05$, far from the maxi-

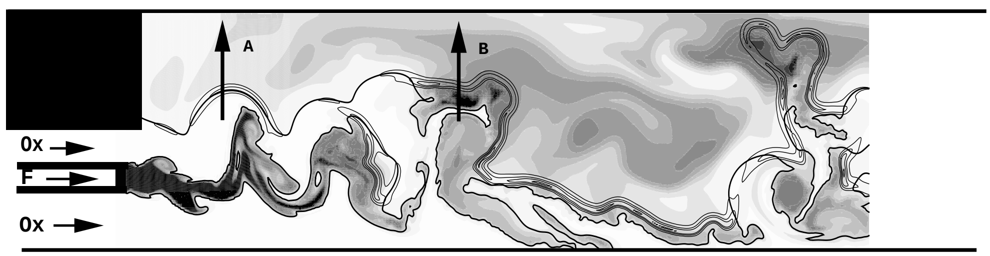

FIGURE 6. Lifted flame (case D): fuel mass fraction Y_F (gray scale) and reaction rate (contour lines) fields are superimposed on the stoichiometric iso-surface (bold lines). Arrows A and B denote locations of cuts displayed in Fig. 7.

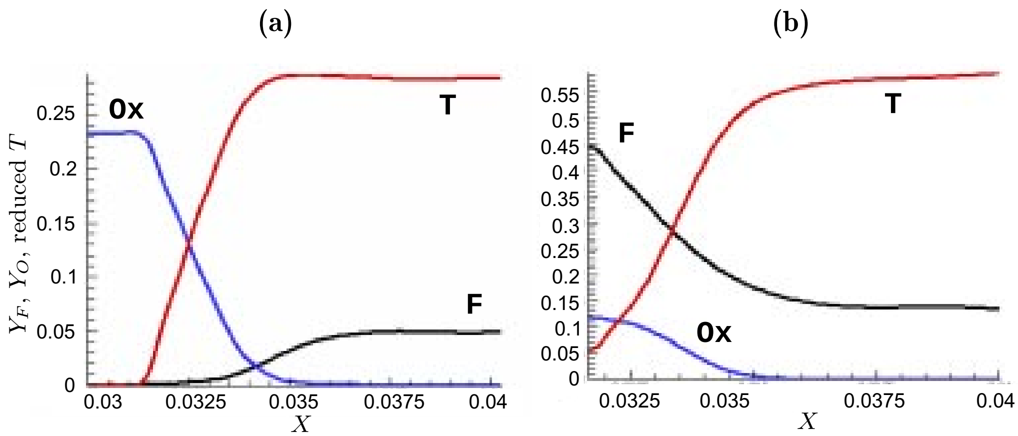

FIGURE 7. Lifted flame (case D): fuel, oxidizer and temperature profiles across the flame front in locations A (left) and B (right) displayed in Fig. 6.

mum value $Y_F = 1$ found in a pure propane/air diffusion flame (the fuel is diluted within burnt gases). The fuel temperature also corresponds to the burnt gases temperature of the previous rich premixed flames. The diffusion flame in location B burns cold oxidizer with a hot mixture of fuel and combustion products. At location B (Fig. 7b), a rich premixed flame is observed: fuel and oxidizer enter the flame front from the same side at a very high equivalence ratio. This premixed flame separates cold fuel/air rich mixture and burnt combustion products.

This occurrence of a rich premixed flame in the flame stabilization process is, *a priori*, surprising but may be easily explained. The mixture fraction z is defined as (Williams (1985)):

$$z = \frac{1}{\Phi + 1}\left(\Phi \frac{Y_F}{Y_F^0} - \frac{Y_O}{Y_O^0} + 1\right) \tag{5.1}$$

where Y_F^0 and Y_O^0 are respectively the fuel and the oxidizer mass fractions in the pure fuel and air streams. $\Phi = sY_F^0/Y_O^0$ is the local equivalence ratio and s the stoichiometric mass coefficient, which corresponds to the mass of oxidizer required to burn a unit mass of fuel. For a propane/air diffusion flame: $Y_F^0 = 1$; $Y_O^0 = 0.23$; $s = 3.64$ and $\Phi = 15.8$. The

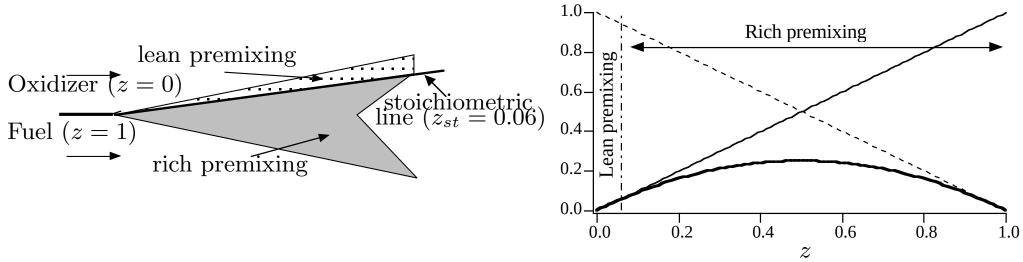

FIGURE 8. Analysis of the rich premixing formation by molecular diffusion when the stoichiometric mixture fraction $z_{st} \approx 0.06$. Left: mixing layer. Right: the fuel (Y_F/Y_F^0; ———), oxidizer (Y_O/Y_O^0; - - - -) and the mixing index ($Y_F Y_O/Y_F^0 Y_O^0$; ━━━) are plotted as a function of the mixture fraction z. The stoichiometric mixture fraction $z_{st} \approx 0.06$ is also indicated (— - —).

mixture fraction z is a passive scalar, unaffected by combustion processes and verifying $z = 0$ in the air stream and $z = 1$ in pure propane streams.

Molecular mixing between air ($z = 0$) and propane ($z = 1$) streams occurs around the intermediate z-level $z = 0.5$, but reactants are in stoichiometric proportions when the mixture fraction takes the value $z_{st} = 1/(\Phi + 1) \approx 0.06$ (for usual hydrocarbons, the stoichiometric value z_{st} is strongly shifted towards the oxidizer stream). Mixtures are lean when $0 < z \leq z_{st} \approx 0.06$ but rich for $z_{st} \approx 0.06 \leq z < 1$. Accordingly, most of the premixed reactants correspond to rich mixtures. This point is illustrated in Fig. 8. Of course, this analysis holds only at a local level when mixing is controlled by molecular diffusion between pure oxidizer and fuel streams. If all of the reactants injected into the combustor chamber perfectly mix before burning, the mixture equivalent ratio would be the global equivalence ratio ϕ.

The LES data can also be averaged in order to be compared to measurements. Fig. 9 shows mean fuel mass fraction, temperature, and reaction rate fields: the reaction rate field confirms that the flame is lifted and stabilized in the vicinity of the recirculation zone. This zone contains hot gases and acts as a heat tank providing the energy required to stabilize the flame. The fuel mass fraction field shows that the leakage of fuel towards the recirculation zone due to the previous burning of rich mixtures appears even on the mean flow.

5.3. *Blow-off (Case E)*

Starting from operating conditions of point D where a lifted flame was observed (Fig. 2), a computation is performed increasing the air flow rate to reach the regime E (see Table 1 and Fig. 2). Very rapidly, after a time of about 20 ms, the fresh air entering the combustion chamber dilutes the mixture involved in rich premixed flames (Fig. 10) and starts filling and cooling the recirculation zone. As soon as this zone is too cold, the whole stabilization process is compromised and the flame quenches as seen in the last snapshots of Fig. 10 where the hot gases are convected towards the burner exhaust while the combustor is filled with premixed cold reactants. This test confirms that blow-off can be predicted with the DTF model (usual simple flamelet models cannot predict blow-off because the flame is generally assumed to burn in a steady state regime). Moreover, this blow-off is found for flow rate values corresponding to experimental observations. Of course, more tests are required to determine the exact quenching limits and to validate the DTF model, but this finding is very promising.

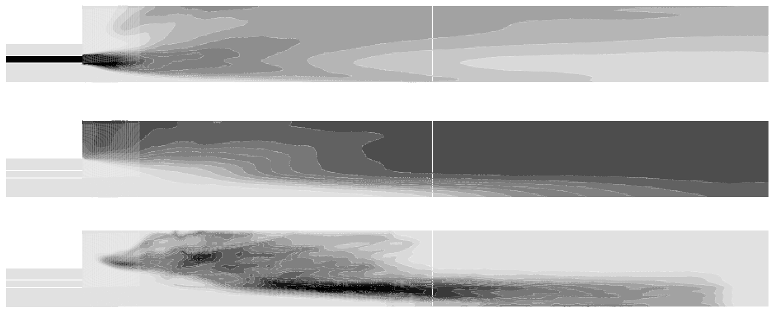

FIGURE 9. From top to bottom, averaged fuel mass fraction, temperature, and reaction rate fields for case D (lifted flame).

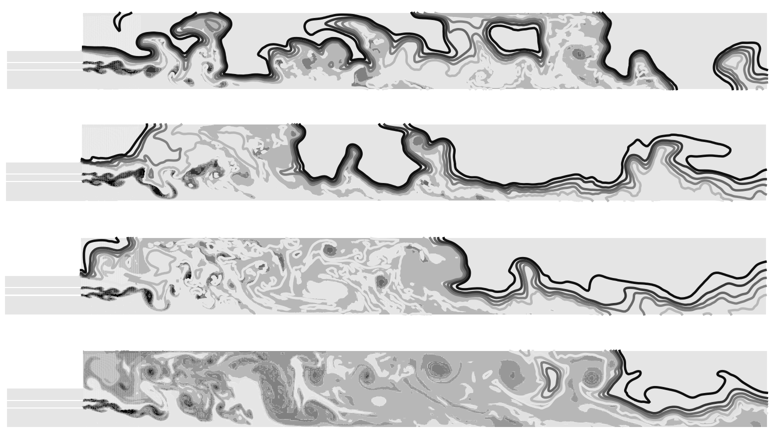

FIGURE 10. Blow-off description. Starting from operating conditions of point D (established lifted flame), the air flow rate is increased to reach the point E conditions (see Fig. 2). Mixing index $Y_F Y_O$ (gray scale) and temperature (contour lines) fields are displayed for four successive instants from top to bottom. The burner is progressively filled with cold premixing and the flame blows off.

6. Conclusions

A dynamic thickened flame (DTF) model is developed for large eddy simulations of turbulent reacting flows and is tested against experimental data. This model extends the thickened flame model (TF) developed by Angelberger *et al.* (1998) and Colin *et al.* (2000a) from the pioneering work of Butler & O' Rourke (1977). In the DTF model, the thickening factor F is larger than unity only in reaction zones, and diffusion processes without chemical reactions are not affected. Accordingly, the DTF model is expected to be suited to situations where non-premixed, partially premixed, and perfectly premixed flames are encountered such as lean premixed prevaporized (LPP) combustors developing for gas turbines.

The DTF model implemented is the AVBP code of CERFACS, and numerical results are compared to experimental data obtained in a turbulent propane/air non-premixed burner at Ecole Centrale Paris (France). This burner exhibits various regimes ("anchored", "lifted", and "extinction") recovered in numerical simulations. In the so-called "lifted" flame regime, the numerical simulations show that combustion mainly occurs in rich premixed flames stabilized by the recirculation zone acting as a hot gases tank. This finding is *a priori* surprising but is in agreement with a simple physical analysis: when propane and air are mixed by molecular diffusion without combustion, most of the premixing corresponds to rich mixtures (fuel in excess) because the stoichiometric iso-surface is strongly shifted towards pure oxidizer for usual stoichiometric flames ($z_{st} \approx 0.06$ when mixing develops around $z \approx 0.5$). Some diffusion flames are also observed but do not correspond to usual flamelets because cold oxidizer burns with a hot mixture of fuel and combustion products. Accordingly, usual flamelet models are not adapted to correctly predict such of lifted flame regimes.

Numerical results are very promising, but further validations against precise instantaneous and averaged experimental data, not yet available, are required.

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