Large eddy simulation of combustion instabilities in turbulent premixed burners

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1. Motivations and objectives

Large Eddy Simulation (LES) techniques are viewed today as the next step in Computational Fluid Dynamics studies to address classes of problems where classical Reynolds-averaged Navier Stokes approaches (RANS) have proved to lack precision or where the intrinsically unsteady nature of the flow makes RANS clearly inadequate. In the field of combustion, the understanding and the control of combustion instabilities are domains where LES is required and will be applied in practical systems. There are at least two reasons for this:

1. Reacting flows submitted to instabilities are dominated by very large eddies sweeping the combustion chamber. Such flows are obviously fully unsteady and make RANS approaches difficult to use.

2. Structures controlling combustion in these flows are large, and LES should be easier in such cases than for turbulent combustion in general where an extended range of eddies has to be resolved to characterize the turbulence/chemistry interaction.

Multiple techniques have been proposed in the past to perform LES of turbulent premixed combustion (Menon and Kerstein 1992, Menon et al. 1994, Smith and Menon 1996, 1997, Piana et al. 1996, 1997, Veynante and Poinsot 1997a). Few of them have been used in a realistic configuration (see for example Kailasanath et al. 1991). In most cases, fundamental studies in simple configurations such as freely propagating flames or stagnation point flames have been performed. In such situations, assumptions are generally made in the fundamental studies (e.g., ignition and quenching mechanisms are ignored) but must be reconsidered in more realistic configurations. Flame stabilization and flame-wall interactions, for example, should be considered in detail and may influence the choice of the LES formulation.

We will briefly recall the basis of LES techniques for combustion and investigate in more detail the performance of one specific method: the Thickened Flame approach, proposed by Butler & O’Rourke (1977). Our objective is to test this method in a configuration where combustion instabilities occur: the flame stabilized behind a backward-facing step. This configuration was chosen since results from many experimental studies are available (Keller et al. 1981, Poinsot et al. 1987) and since the configuration contains many features in common with real combustion chambers. Our attention will be also focused on flame stabilization and flame-wall interaction.

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These issues have been addressed previously using DNS and RANS approaches (Poinsot 1996, Poinsot et al. 1996, Bruneaux et al. 1996) but have not received much attention in the context of LES. Our first goal is to propose a LES technique which correctly reproduces flame wrinkling, at least when the flow is dominated by large structures, and handles flame-wall interactions and stabilization regions in a physical manner without ad hoc corrections.

The different techniques proposed for LES of premixed combustion will be briefly summarized in Section 2. Our decision to investigate the thickened flame (TF) model, initially proposed by O’Rourke and his coworkers (Butler & O’Rourke 1977, O’Rourke & Bracco 1979), will be explained.

Section 3 will present the configuration studied and Section 4 the numerical code and the boundary conditions. The stabilization studies are described in Section 5, and Section 6 presents flame response to inlet velocity fluctuations. The effect of numerical parameters controlling this response (LES treatment, perturbation amplitude, thermal conditions on inlet sections) is also discussed.

2. LES techniques for turbulent premixed combustion

2.1 LES framework for combustion

Assuming that $G$ is the LES filter and $x$ the location, any filtered quantity $\overline{Q}$ is defined as:

$$\overline{Q}(x, t) = \int_{-\infty}^{+\infty} Q(x, t') G(x - x') dx'$$

(1)

For reacting flows, a Favre filtering is defined as:

$$\overline{\rho Q} = \overline{\rho Q} = \int_{-\infty}^{+\infty} \rho Q(x, t) G(x - x') dx'$$

(2)

where $\overline{Q}$ is the filtered density. The previous definition is similar to Favre averaging, widely used in RANS context.

Filtering the conservation equations controlling reacting flows introduces unknown quantities to be modeled: (1) $\overline{u_i u_j} - \overline{u_i u_j}$, the unresolved Reynolds stresses, which requires a subgrid scale turbulence model; (2) $\overline{u_i Y_k} - \overline{u_i Y_k}$, the unresolved species fluxes, where a simple gradient expression is usually assumed:

$$\overline{u_i Y_k} - \overline{u_i Y_k} = -\nu_T \frac{\partial \overline{Y_k}}{\partial x_i}$$

(3)

with $\nu_T$ the subgrid kinematic turbulent viscosity and $S_c$ the turbulent Schmidt number; (3) $\overline{u_i T} - \overline{u_i T}$, the unresolved heat fluxes, also modeled by a gradient expression; (4) $\overline{Y_k T} - \overline{Y_k T}$ and $\overline{Y_k T^n} - \overline{Y_k T^n}$, the species-temperature correlations, occurring when specific heats $C_p$ are expressed in terms of polynomial approximations of $T$, which are usually neglected; and (5) the filtered reaction rate $\overline{\omega_k}$.

In the following, our attention will be focused on modeling the filtered reaction rate $\overline{\omega_k}$. The other terms have been addressed in previous studies. The Reynolds
stresses are generally described using Smagorinsky or Germano dynamic models whereas unresolved turbulent transports are expressed with gradient expressions. No attempt has been yet conducted to take into account counter-gradient transport evidenced by theory (Libby & Bray 1981, Bray et al. 1989) or DNS (Veynante et al. 1996, Veynante & Poinsot 1997b) in LES.

One difficulty is encountered for large eddy simulations of premixed flames: the flame thickness $\delta_l^f$ is in the range of approximately 0.1 to 1.0 mm and is generally smaller than the LES mesh size $\Delta$. Accordingly, species mass fraction and temperature profiles are very stiff variables, thus the flame front cannot be resolved on the computational mesh. To overcome this difficulty, two main approaches have been proposed: simulation of an artificially thickened flame (TF) or use of a flame front tracking technique ($G$-equation).

2.1 Arrhenius law based on filtered quantities (Arrhenius model)

A first simple model is to neglect subgrid scale contributions and to write the reaction rate as an Arrhenius law for filtered quantities:

$$\overline{\omega}_F = \overline{A} \overline{Y}_F^a \overline{Y}_O^b \exp \left( -\frac{T_a}{T} \right)$$

(4)

Such simple expressions assume perfect mixing at subgrid scales and implicitly assume that turbulent time scales, $\tau_t$, are shorter than chemical time scales, $\tau_c$ ($\tau_t \ll \tau_c$). The reaction zone thickness is also assumed sufficiently large to be resolved on the LES mesh size. This formulation is generally used for reacting flows in atmospheric boundary layers (Nieuwstadt, 1997) but is not relevant in most combustion applications. Segregation factors may be also introduced to correct Arrhenius expression to account for unmixedness. Specific Arrhenius-type expressions incorporating combustion delays and changes due to subgrid scale mixing may also be derived in an ad-hoc manner, for example Kailasanath (1985,1991).

2.2 The field equation ($G$ model)

In this approach (Kerstein et al., 1988), the flame surface is described as an infinitely thin propagating surface (i.e. flamelet). In using this approach, one tracks the position of the flame front using a field variable $G$. The flame surface is associated with a specific isolevel $G = G^*$. The gradients in the $G$-field can be much smoother than those of the progress variable $c$ to the point where they can be resolved on the LES mesh. Work in progress on the use of $G$ equation has shown the potential but also the difficulties of this approach (see Bourlioux et al.1996; Piana et al.1996, 1997, Im et al.1996, Veynante and Poinsot 1997a).

2.3 Random vortex methods (RVM model)

Random vortex methods are another class of models suitable for LES of premixed combustion. In this grid-free approach, chemistry may be handled in a Lagrangian manner by following flame elements. Examples of such approaches may be found in Ghoniem et al.(1988, 1992).
2.4 The thickened flame model (TF model)

The key idea of the thickened flame (TF) model is to consider a flame having the same laminar flame speed $s_l$ but a larger flame thickness than the actual actual flame in order to be resolved on the LES computational grid (Butler and O'Rourke 1977, O'Rourke and Bracco 1979). Following simple theories of laminar premixed flame (Williams 1985, Kuo 1986), the flame speed $s_l$ and the flame thickness $\delta_l$ may be expressed as:

$$s_l \propto \sqrt{a \dot{W}} \quad ; \quad \delta_l \propto \frac{a}{s_l}$$

where $a$ is the thermal diffusivity and $\dot{W}$ the total reaction rate. Then, an increase of the flame thickness $\delta_l^0$ by a factor $F$ while maintaining a constant flame speed $s_l^0$ may be achieved by replacing the thermal diffusivity $a$ by $F a$ and the reaction rate $\dot{W}$ by $\dot{W}/F$ as summarized in Table I. Numerically, such a transformation is performed simply by dividing the pre-exponential constant and the Prandtl and the Schmidt numbers by the thickening factor $F$.

<table>
<thead>
<tr>
<th>Flame speed</th>
<th>Flame thickness</th>
<th>Preexponential</th>
<th>Prandtl</th>
<th>Schmidt Factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal flame $s_l^0$, $\delta_l^0$</td>
<td>$A^0$, $P_r^0$, $S_c^0$</td>
<td>$A^1 = A^0/F$, $P_r^0/F$, $S_c^0/F$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table I: Comparison between normal (superscript 0) and thickened flame (superscript 1). The thickening factor is $F$.

For sufficiently large values of the factor $F$, the thickened flame front may be resolved on the LES computational mesh. In practical applications, values of $\delta_l^0$ (estimated by $\delta_l^0 s_l^0/a \approx 4$) are of the order of 0.2 to 1 mm so that thickening factors $F$ of the order of 3 to 10 should suffice for many practical simulations. Based on Arrhenius law, the TF model has the advantages that it can handle ignition and flame-wall interaction processes without any sub-model.

However, thickening the flame front may have the following two undesired effects. First, the flame propagation may be affected when small scales are present in the flow because these structures could become unable to wrinkle the thickened flame front (Poinsot et al.1991). For combustion instabilities, this drawback may not be crucial because of the large values of the ratio of the vortex size $L$ to the flame thickness $\delta_l^0$. Second, the sensitivity of the flame to stretch is also increased by $F$ because of the transformation. The thickened flame will react to a stretch of $\kappa/F$ as the actual flame would to a stretch of $\kappa$. Many DNS of turbulent premixed combustion have suggested that, in the mean, the effect of stretch on the local flamelets was not strong (Haworth & Poinsot 1992, Baum et al.1994, Trouvé & Poinsot 1994) but increasing this effect by a factor $F$ of the order of 10 may have unexpected effects,
for example on quenching. Note however that this difficulty is also encountered in the $G$-equation approach where strain effects on the displacement speed have to be introduced in an ad-hoc fashion because the $G$ model is, by construction, insensitive to stretch.

3. Objectives and configuration

Our objective in the present work is to investigate the limits of the TF model for large eddy simulations of combustion instabilities in premixed burners. The issues mentioned before will be analyzed by computing the same flow (prototype of a combustion instability in a premixed burner) with both “normal” and a “thickened” flame descriptions. The normal flame is described using a classical DNS formulation. For thickened flame simulations, no LES model is used for the flow itself; our objective is just to qualify the TF approach independently of the LES turbulence model. Furthermore, for the present two-dimensional simulations, no small-scale turbulence is present. These TF simulations are in fact DNS where the flame characteristics have been changed according to the relations summarized in Table I. For future studies in three-dimensional flows, an additional coupling model between the turbulence LES model and the TF model should be incorporated.

Figure 1. Numerical configuration corresponding to the premixed propane/air burner used by Poinso et al. (1987) to investigate combustion instabilities. The actual burner has five injection slots.

The numerical configuration, displayed in Fig. 1, corresponds to the turbulent premixed propane-air experimental burner of Poinso et al. (1987). This burner is dominated by multiple instability modes corresponding to acoustic eigenmodes of the whole combustion system (including compressor and inlet pipes). Observed frequencies range between 440 Hz and 590 Hz. The strongest mode occurs at 530 Hz for an equivalence ratio $\phi$ of 0.92 and a total flow rate $\dot{m}$ of 73 g/s (flow conditions are summarized in Table II).
Table II: Flow conditions for the 530 Hz instability mode (Poinsot et al. 1987). $U_0$ is the inlet velocity, $c_0$ the sound speed. $\nu_0$ is the kinematic viscosity of fresh gases. $l$ and $b$ are respectively the burner and the step thickness (see Fig. 1).

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$s_i^0$</th>
<th>$\delta_i^0$</th>
<th>$U_0$</th>
<th>$c_0$</th>
<th>$Re = c_0l/\nu_0$</th>
<th>$U_0(l - b)/\nu_0$</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.92</td>
<td>0.40</td>
<td>1.1 $10^{-4}$</td>
<td>42</td>
<td>345</td>
<td>$2.1 \times 10^5$</td>
<td>3950</td>
<td>530</td>
</tr>
</tbody>
</table>

For the flow conditions in Table II, the whole system resonates at a frequency of 530 Hz while mushroom-like vortices are shed at the same frequency from all five injection slots. These structures are not created by hydrodynamic instabilities (which are also observed but at a higher frequency) but are due to strong simultaneous velocity surges in the five injection slots. These vortices grow, are convected, and interact with vortices issued from neighboring slots, leading to small-scale turbulence and intense heat release. The time delay between the velocity surge leading to the formation of these vortices and the peak heat release is an essential parameter for all combustion instability models (see Crocco & Cheng 1956, Crocco 1969, McManus et al. 1993, Candel et al. 1996). Estimating this delay does not require one to take into account the whole system and the acoustics which induce the vortex formation itself. A proper strategy is to create a vortex by pulsating the combustion chamber inlet flow field and to study the effect of this vortex on the overall combustion process.

4. Numerical technique and protocol to study flame response

This study is conducted using the NTMIX code, a two-dimensional DNS solver developed by CTR and Ecole Centrale Paris and described in Veynante & Poinsot (1995) or Veynante et al. (1996). The full compressible reacting Navier-Stokes equations are solved assuming perfect gases with constant molar mass and a specific heat ratio $\gamma = 1.4$. The thermal conductivity $\lambda$ and the diffusion coefficient $D$ are obtained from the dynamic viscosity coefficient $\mu$ according to

$$\lambda = \mu C_p / P_r \quad \text{and} \quad D = \mu / (\rho S_c),$$

where the Prandtl number $P_r$ and the Schmidt number $S_c$ are constant. As a consequence the Lewis number $L_e = S_c / P_r$ is also constant. The viscosity $\mu$ is a function of temperature according to $\mu = \mu_u (T / T_u)^n$ where $n = 0.76$.

The computational domain is $L_x \times L_y$ with $N_x \times N_y$ grid points. Boundary conditions (Fig. 1) correspond to a partially blocked inlet (blockage ratio $b/l$ of 85%) on the left, non-reflecting boundary conditions on the right, and symmetric boundaries on both sides. The velocity profile at the inlet is a $tanh$ function with a thickness $\delta_y$.

An important difficulty in studying combustion delays is that excitation procedures have to be performed on a given baseline flow. Either this baseline flow is
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stable and the flame response might not correspond to the one expected for unstable cases, or the baseline flow is unstable and measuring a transfer function becomes extremely difficult because the flow is dominated by its own instability (similar difficulties are encountered for DNS of non-reacting flows in absolutely unstable regimes). Experimentally, the only possible approach is the first solution: Poinso et al. (1986), for example, have measured the reflection coefficient of a premixed flame but only for stable regimes close to instability. Numerically, however, it is possible in certain cases to create a stable baseline flow in a regime which should be unstable by slightly changing the expression of the reaction rate. Indeed, theoretical studies of combustion instabilities indicate that one main factor promoting instabilities is the dependence of the reaction rate on pressure (i.e. on density) as evidenced by the Rayleigh criterion which states that instability occurs when pressure and total heat release oscillate in phase (Crocco 1956, McManus et al. 1993). Poinsot and Candel (1988), for example, verified numerically that an anchored flame was more likely to become unstable when flame speeds were pressure dependent. This suggests the following approach. Assuming that fuel is the deficient species controlling the reaction rate \( \dot{\omega}_F \):

\[
\dot{\omega}_F = B \rho Y_F \exp \left( -\frac{T_a}{T} \right)
\]  

(6)

then for the pressure sensitive (PS) case, any pressure increase (corresponding to an increase of the density \( \rho \)) will also increase the reaction rate. To inhibit this effect, a second expression called PI (pressure insensitive) is also used:

\[
\dot{\omega}_F = B \frac{P_0}{r T} Y_F \exp \left( -\frac{T_a}{T} \right)
\]  

(7)

where \( P_0 \) is a constant reference pressure. The PI expression makes the reaction rate insensitive to pressure waves and cuts an important link in the combustion instability loop.

The PS and PI expression will give the same results for a stable flame (for example, an unconfined flame). However, only the PI expression can produce a stable baseline flow in ducted flows.

5. Stabilization and baseline flows for ducted flames

The different runs presented in this report are summarized in Table III. Runs B2, S4, S5 and S7 correspond to DNS (flames with normal thickness \( \delta_0 \)) while runs M1, S3, S6, and S9 correspond to thickened flames (by a factor \( F \) ranging from 2.5 to 7.5). Runs B2, M1, S6, and S9 correspond to the same physical flow (\( Re = 75000 \)) where the computation is performed with DNS for B2 (\( F = 1 \)) and with various values of the thickening factor \( F \): 2.5 (M1), 5 (S6), and 7.5 (S9). Runs S4, S5, and S7 correspond to DNS with a lower Reynolds number (\( Re = 15000 \)). Two thermal conditions have been tested for the blockage wall lying between \( y = 0 \) and \( y = b \) at the inlet (Fig. 1). This wall may be adiabatic (adiabatic wall, called AW) or cooled
with an imposed temperature $T_w = T_1$ where $T_1$ is the inlet gases temperature (cooled wall, called CW in Table III).

Table III: Flow conditions for the DNS and LES of ducted flames. For all flows: $U_0/c_0 = 0.1$; the Reynolds number $Re$ is $= c_0l/\nu_0$; the temperature change through the flame front is $T_2/T_1 = 4$ ($\alpha = (T_2 - T_1)/T_2 = 0.75$); the sound speed in the fresh gas is $c_0$ (and $2c_0$ in the burnt gas); the activation temperature $T_a$ is such that $\beta = \alpha T_a/T_2 = 7$; the box height is $l/L = 1$; the flame Mach number $s_0^0/c_0$ is $0.0032$; the blockage is $0.85 \ (b/l = 0.85)$. $\delta_1$ is the flame thickness after thickening ($\delta_1 = F \delta_0$).

<table>
<thead>
<tr>
<th>RUN</th>
<th>$l/\delta_1$</th>
<th>$Re$</th>
<th>$F$</th>
<th>RR</th>
<th>Wall cond.</th>
<th>$\delta_Y/l$ cond.</th>
<th>$X_{max}/l$</th>
<th>$N_x$</th>
<th>$N_y$</th>
</tr>
</thead>
<tbody>
<tr>
<td>S3</td>
<td>9.6</td>
<td>75000</td>
<td>5</td>
<td>PS</td>
<td>AW</td>
<td>0.03</td>
<td>9</td>
<td>150</td>
<td>64</td>
</tr>
<tr>
<td>S4</td>
<td>9.6</td>
<td>15000</td>
<td>1</td>
<td>PI</td>
<td>CW</td>
<td>0.01</td>
<td>9</td>
<td>150</td>
<td>64</td>
</tr>
<tr>
<td>S5</td>
<td>9.6</td>
<td>15000</td>
<td>1</td>
<td>PI</td>
<td>CW</td>
<td>0.01</td>
<td>12</td>
<td>200</td>
<td>64</td>
</tr>
<tr>
<td>S6</td>
<td>9.6</td>
<td>75000</td>
<td>5</td>
<td>PI</td>
<td>AW</td>
<td>0.03</td>
<td>9</td>
<td>150</td>
<td>64</td>
</tr>
<tr>
<td>S7</td>
<td>9.6</td>
<td>15000</td>
<td>1</td>
<td>PI</td>
<td>AW</td>
<td>0.01</td>
<td>9</td>
<td>150</td>
<td>64</td>
</tr>
<tr>
<td>S9</td>
<td>6.4</td>
<td>75000</td>
<td>7.5</td>
<td>PI</td>
<td>AW</td>
<td>0.03</td>
<td>9</td>
<td>150</td>
<td>64</td>
</tr>
<tr>
<td>M1</td>
<td>19.2</td>
<td>75000</td>
<td>2.5</td>
<td>PI</td>
<td>AW</td>
<td>0.03</td>
<td>9</td>
<td>300</td>
<td>128</td>
</tr>
<tr>
<td>B2</td>
<td>48</td>
<td>75000</td>
<td>1</td>
<td>PI</td>
<td>AW</td>
<td>0.03</td>
<td>750</td>
<td>300</td>
<td></td>
</tr>
</tbody>
</table>

These conditions do not correspond exactly to the experiment of Poinset et al. Although the geometry is the same, the Reynolds number of the largest simulation (B2) is only one third of the experiment. Our goal, however, is to validate the TF methodology and, for the moment, no detailed comparisons are performed with the experiment.

5.1 Effects of formulations of $\dot{\omega}$ on stabilization

All computations are initialized with an oblique flame starting behind the step using temperature and fuel mass fraction profiles corresponding to a one-dimensional laminar premixed flame for the same equivalence ratio. Starting from this field, the simulation evolves without external excitation until a steady state is reached or when a well established oscillation is found. Figure 2 compares the temporal evolution of the total reaction rate for PS and PI formulations in cases S3 and S6. The PS formulation leads to oscillations both in transverse ($f_l/c_0 \simeq 1$) and longitudinal modes ($f_l/c_0 \simeq 18$) of the computational box. On the other hand, the PI formulation leads to a constant reaction rate and a steady flame regime.

5.2 Effect of inlet wall thermal condition

Figure 3 shows velocity vectors and the reaction rate field for run S5 in the vicinity of the injection slots. This flow exhibits a recirculation zone having a length of about 7.7b. The gas temperature inside this recirculation zone controls the anchoring of
**Figure 2.** Effect of reaction rate formulation on flow stabilization: (a) case S6: pressure insensitive form; (b) case S3: pressure sensitive form. Time evolution of total burning rate (adiabatic walls).

**Figure 3.** Zoom on velocity vectors and reaction rate field in the vicinity of the injection slot (Cold Wall - run S4).
the flame. These hot gases are produced by combustion and recirculated behind
the step but may also be cooled by the wall. Therefore the thermal conditions on
the wall between \( y = 0 \) and \( y = b \) are important parameters (see Fig. 1).

Any heat losses in the vicinity of the recirculation gas have a strong effect on the
steady flame position but also on its response to unsteady pulsations. Two thermal
conditions have been tested for this wall. The adiabatic wall (AW) condition (run
S7) allows the flame to start on the wall while the cooled wall (CW) condition
(run S4) inhibits reaction near the wall and forces the flame to be lifted as shown
by the reaction rate fields in Fig. 4. The flame length is also increased and the
characteristic flame time is changed (see next Section).

6. Transfer function of premixed ducted flames

6.1 Methodology

Once stable flames are obtained, their transfer function may be studied by injecting
acoustic disturbances through the inlet. The inlet velocity profile is modulated
here according to the following expression:

\[
U(x, y, t) = U_{\text{steady}} \left( 1 + U_{\text{inc}}^+ \exp \left[ - \left( \frac{t - t_{\text{trig}}}{t_{\text{width}}} \right)^2 \right] \right)
\] (8)

Examples of a flame excited with \( U_{\text{inc}}^+ = 1, U_0 t_{\text{trig}}/l = 0.5 \) and \( U_0 t_{\text{width}}/l = 0.6 \)
are displayed in Fig. 5 for run S6 (see table III). The formation of a large reacting
vortex is observed. The shape of this vortex is similar to the mushroom vortices
observed in the experiment of Poinson et al.(1987). Because of the AW condition
used for the wall, the flame remains anchored at all times on the wall.

Figure 6 shows that the total heat release lags the inlet flow rate by a delay
\( \tau \simeq 2.5l/U_0 \). This delay directly controls the instability modes since the period \( T \)
of most combustion instabilities is of the order of \( 2\tau \) (Crocco & Cheng 1956, Poinson
et al.1987). However, the delay obtained through such a simulation must be used
with caution because it depends on multiple parameters. In the following, three
parameters will be investigated: (1) the thickening parameter \( F \) of the TF model,
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Figure 5. Pulsated premixed flame (S6) computed using the TF model (thickening factor $F = 5$). Temperature field. (a) $U_0t/l = 0.8$, (b) $U_0t/l = 1.6$, (c) $U_0t/l = 2.4$.

Figure 6. Time evolution of inlet flow rate (---), total reaction rate (---) and outlet flow rate (-----). Run S6 with $F = 5$. 
corresponding to the LES treatment of the reaction rate, (2) the wall condition (cold or adiabatic), and (3) the excitation amplitude $U_{inc}^+$.

### 6.2 Effects of LES treatment (thickening factor $F$)

The $Re = 75000$ case was computed with thickening factors $F = 1$ (run B2, 750 \times \text{grid 300 points}), $F = 2.5$ (M1, 300 \times 128 points), $F = 5$ (S6, 150 \times 64 points) and $F = 7.5$ (S9, 150 \times 64 points). As the flame becomes larger ($F$ is increased), the grid size $N_x \times N_y$ may be reduced, decreasing the computational time. The excitation parameters are $U_{inc}^+ = 1$, $U_0 t_{trig} / l = 0.5$ and $U_0 t_{width} / l = 0.6$. Figure 7 shows the time evolution of the total reaction rate for these four simulations.

![Figure 7](image)

**Figure 7.** Effects of the thickening factor $F$ (LES treatment of the reaction rate). The normalized total burning rate is displayed versus time. Comparison between DNS, $F = 1$ (run B1, -----), LES with $F = 2.5$ (M1, ------), $F = 5$ (S6, -----) and $F = 7.5$ (S9, --------). Excitation parameters are $U_{inc}^+ = 1$, $U_0 t_{trig} / l = 0.5$ and $U_0 t_{width} / l = 0.6$.

The general evolution of all flows is similar: differences of the order of 20% are observed for the total reaction rate. However the shapes of the reaction rate curves are different: the DNS ($F = 1$) burns initially faster than the LES cases but more slowly in the late stages of the interaction. This finding is consistent with the TF formalism: less flame surface is created for LES runs than for DNS, leading to a reduced combustion, because the sensitivity of a thickened flame to a hydrodynamic perturbation is lower than the one of a thin flame as shown by Poinset et al. (1991). Later on, however, the additive reactants injected during the excitation have to burn, leading to a larger combustion rate in the LES computations.

Figures 8 and 9 display fields of instantaneous reaction rates for the four computations at times $U_0 t / l = 1.6$ and $U_0 t / l = 2.8$, respectively. These plots confirm the thickening of the reaction zone when the factor $F$ is increased. This thickening affects flame wrinkling in complex ways: the DNS creates a first pocket of fresh gases
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in the burnt products earlier than the three LES runs. More flame surface is also generated. This flame surface is mainly due to small scale wrinkling, which leads to the formation of small pockets. These pockets are burned out rapidly. On the other hand, less small pockets are initially created in the LES cases so that a large pocket of fresh reactants is consumed later. This phenomenon becomes dramatic for the $F = 7.5$ LES run where the evolution of the flow after $U_0 t/l = 1$ differs from the DNS result by 30% because most of the flame wrinkling is missed.

Figure 8. Instantaneous reaction rate fields at time $U_0 t/l = 1.6$. Comparison between DNS (a), LES with $F = 2.5$ (b), LES with $F = 5$ (c) and LES with $F = 7.5$ (d). See caption of Fig. 7 for runs characteristics.

6.3 Effects of inlet wall condition

Figure 10 compares two DNS simulations (runs S5 and S7) for an excitation corresponding to $U_{inc}^+ = 1$, $U_{trig}/l = 1.5$ and $U_{width}/l = 0.6$. Run S5 is similar to S4 (only the box length is different) and performed with a cold wall (CW) condition on the inlet wall while S7 assumes an adiabatic wall (Reaction rate contours for both flames under steady conditions are displayed on Fig. 4).

Figures 11 and 12 display fields of reaction rates for these two computations at reduced times $U_0 t/l = 2.4, 3.6, 4.8$ and 6. The flame stabilized behind a cold
Figure 9. Instantaneous reaction rate fields at time $U_0 t/l = 2.8$. Comparison between DNS (a), LES with $F = 2.5$ (b), LES with $F = 5$ (c) and LES with $F = 7.5$ (d). See caption of Fig. 7 for runs characteristics.

wall (Fig. 12) reacts later to excitation than the adiabatic flame (Fig. 11) but more strongly. Large differences both in delay and amplitude are observed, demonstrating the importance of the condition chosen for the inlet wall. Two factors explain these differences: (1) the CW flame lies closer to the recirculating burnt region than the AW flame and, therefore, ‘feels’ the vortex with less amplitude and at a later time than the AW flame, and (2) the reaction rate of the CW flame is very small near the injection slot because of heat losses while the AW flame burns everywhere with the laminar flame speed. The resulting pattern of this ‘flame-vortex’ interaction is, therefore, extremely different. The effects of this boundary condition appear to be as strong as the thickening factor $F$ used in the TF model. This shows that the LES of the purely propagating flame (handled with the TF model) is only one aspect of CFD for combustion instabilities of confined flames and that factors such as boundary conditions and flame stabilization could play a crucial role.

LES with cold wall conditions are not presented here because specific treatments of wall heat fluxes will be required for these cases. Dividing $P_r$ by a factor $F$ thickens the flame but also increases heat transfer to the walls by the same factor.
Figure 10. Effects on inlet wall condition. Normalized total burning rate versus time. Comparison between adiabatic wall (AW - S7) and cold wall (CW - S5).

Figure 11. Fields of reaction rate for simulation S7 (DNS, adiabatic wall): (a) $U_0t/l = 2.4$, (b) $U_0t/l = 3.6$, (c) $U_0t/l = 4.8$ and (d) $U_0t/l = 6$. 
Figure 12. Fields of reaction rate for simulation S5 (DNS, cold wall): (a) $U_0 t/l = 2.4$, (b) $U_0 t/l = 3.6$, (c) $U_0 t/l = 4.8$ and (d) $U_0 t/l = 6$.

This could be avoided by an adequate treatment of wall fluxes but remains to be investigated.

6.4 Effects of excitation amplitude

Most models for combustion instability are linear. It is, however, well-known that flame response is strongly non-linear, and the excitation amplitude to pulsate flames has to be chosen carefully. Figure 13 shows flame response for an LES run (S6, $F = 5$) for three excitation levels: $U_{inc}^+ = 0.1$, 0.5, and 1. In all cases, $U_0 t_{trig}/l = 0.5$ and $U_0 t_{wsi, dilk}/l = 0.6$. For low levels of excitation amplitude (10% of incoming velocity for $U_{inc}^+ = 0.1$), the delay is much longer than it is in cases with more intense perturbations. Examination of the instantaneous flow fields reveals that no pocket is formed for case $U_{inc}^+ = 0.1$. Flame wrinkling is higher in the two other cases where the flame is shred by the vortical field.

6.5 Theoretical analysis of the thickened flame response

The response of a thickened flame to an excitation is now analyzed. Our objective is to propose a simple model explaining the findings of Fig. 7 and 13. Under the flamelet assumption, the flame stretch $K$ measures the increase in flame surface area $A$ (Candel & Poinsot, 1991):

$$K = \frac{1}{A} \frac{dA}{dt}$$ (9)
Figure 13. Effects of excitation amplitude. Normalized total burning rate versus time for $U_{inc}^+ = 0.1$ (---), $U_{inc}^+ = 0.5$ (----) and $U_{inc}^+ = 1$ (---). Run S6 ($F = 5$).

Figure 14. Analysis of the initial flame response. The normalized total burning rate is displayed versus time. Bold lines correspond to numerical results (already displayed on Fig. 7), thin lines (-----) are fits according to Eq. (10). DNS, $F = 1$ (run B1, ---), LES with $F = 2.5$ (M1, ----), $F = 5$ (S6, ······) and $F = 7.5$ (S9, ······). Excitation parameters are $U_{inc}^+ = 1$, $U_0 t_{trig}/l = 0.5$ and $U_0 t_{width}/l = 0.6$. 
Assuming that the local reaction rate per unit of flame surface area is almost constant along the flame front, the total reaction rate $\dot{W}$ is proportional to the flame area $A$ and depends on the mean stretch in the same way.

In our simulations, the mean stretch is mainly due to the strain $\kappa$, which is in turn due to the vortex generated by the inlet velocity perturbation. But, following Meneveau and Poinset (1990), an efficiency function $C$ depending on the ratio between the vortex size $r$ and the flame thickness $\delta_l$ has to be introduced to take into account the reduced ability of small vortices to wrinkle the flame front. Then, integrating Eq. (9) leads to an estimate of the time evolution of the reduced total reaction rate $\dot{W}/\dot{W}_0$, where $\dot{W}_0$ corresponds to the total reaction rate under steady state operation:

$$\frac{\dot{W}}{\dot{W}_0} = \exp \left[ C \left( \frac{r}{\delta_l} \right) \kappa t \right]$$ \hspace{1cm} (10)

Estimates of the vortex size $r$ and the strain rate $\kappa$ are now required. One may propose:

$$r \approx U_0 t_{width} \quad ; \quad \kappa \approx U^+_{inc} \frac{U_0}{r}$$ \hspace{1cm} (11)

The efficiency function $C(r/\delta_l)$ may now be estimated by fitting the expression (10) on reduced reaction rates displayed on Fig. 7 and 13. Reaction rate fits are displayed against numerical simulations on Fig. 14 (Only the growing phase of the total reaction rate is used here). The agreement is quite satisfactory. On Fig. 15, the efficiency function $C(r/\delta_l)$ is plotted as a function of the length scale ratio $r/\delta_l$ and compared to the efficiency function $C_{MP}$ proposed by Meneveau and Poinset.
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and extracted from the flame-vortex interaction DNS conducted by Poinset et al. (1991). As expected, the efficiency function $C$ is found to decrease with the length scale ratio $r/\delta_1$ with a shape similar to $C_{MP}$. The discrepancy between $C$ and $C_{MP}$ is probably due to the difference between present simulations and those of Poinset et al. (two vortices interacting with a normal flame in Poinset et al. DNS, one velocity perturbation interacting with an oblique flame here), leading to differences in the estimation of $r$ and $\kappa$. Another point is that, in our simulation, the flame structure is modified by decreasing the pre-exponential factor $B$ and the Schmidt number $S_c$, keeping the hydrodynamic perturbation constant. In the simulations of Poinset et al., the flame structure remains unchanged whereas vortex size and strength are modified. Nevertheless, this finding is very interesting because the efficiency function $C(r/\delta_1)$, and more generally an ITNFS-like formulation (see Meneveau and Poinset, 1991), could be implemented in the reaction rate expression to correct the reduced ability of a thickened flame to be wrinkled by small structures. This point could be investigated from DNS of flame-vortex interactions using various values of the thickening factor $F$.

7. Conclusion

The forced response of a flame stabilized behind a step in a geometry corresponding to the experiment of Poinset et al. (1987) has been studied at different Reynolds numbers using Direct Numerical Simulations and Large Eddy Simulations based on the Thickened Flame model. This model allows the computation of a premixed flame on a coarse grid by increasing its thickness while maintaining its flame speed. The TF model is able to compute the flame response within 20% when thickening factors as large as 5 are used. Even though the TF model modifies the flame response, its influence is smaller than other parameters which are specifically linked to combustion instabilities in dump-stabilized flames: the excitation amplitude and the thermal condition on the wall near the injection slot, for example, are found to have comparable effects on the flame response. An efficiency function, similar to the ITNFS formulation proposed by Meneveau and Poinset (1991), could be introduced to reduce the modification of the flame response due to the TF model. Accordingly, the thickened flame (TF) approach seems to be a good compromise for large eddy simulations of combustion instability in premixed burners.

REFERENCES


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