Influence of boundary conditions in LES of premixed combustion instabilities

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1. Motivations and objectives

Large eddy simulation (LES) techniques are often presented today as the ideal tool to address combustion instabilities problems. Combustion instabilities have been studied for a long time (Crocco 1956, 1969, Poinsot and Candel 1988, Candel *et al.* 1996), but their prediction during the design process of real systems remains extremely difficult. The recent progress of direct numerical simulations (DNS) (Poinsot, Candel and Trouvé 1996) and of LES for reacting flows (Veynante and Poinsot 1997) suggests that such prediction should be easier in the near future. One important reason for this is the fact that very large scale structures control combustion instabilities (Poinsot *et al.* 1987); for these scales, LES should perform better than for 'stable' turbulent combustion (Bray *et al.* 1989, Baum *et al.* 1994) where an extended range of eddies has to be resolved to characterize the turbulence/chemistry interaction.

To develop LES techniques for realistic computations of combustion instabilities, the following issues must be addressed:

- LES models must be developed both for the flow and for the flow/chemistry interaction. These goals are the center of current research efforts (Menon and Kerstein 1992, Menon *et al.* 1994, Moser and Klein 1996, Smith and Menon 1996, 1997, Im *et al.* 1996, Piana *et al.* 1996, 1997, Veynante and Poinsot 1997a,b, Angelberger *et al.* 1998, Boger *et al.* 1998) that will not be described here. We will use both the ICC methodology proposed by Bedat *et al.* (1997, 1999) and Angelberger *et al.* (1998) to describe chemistry and the thickened flame model to describe flame chemistry interaction (O'Rourke and Bracco 1979, Butler and O'Rourke 1977, Veynante and Poinsot *et al.* 1997).
- The models for flow and combustion must be implemented in a code able to handle the complex geometries of real burners. At the present time, this means using an unstructured grid code able to compute reacting flows on hybrid meshes. For the present work, we used a hybrid mesh code called AVBP and developed at CERFACS which is built upon a parallel library called COUPL (produced jointly by CERFACS and Oxford University) (Nicoud *et al.* 1996, Ducros *et al.* 1997). The geometry employed for the present study is typical of burners found in real gas turbines used for energy production.
- The specific points emphasized in the present paper are linked to the initial and boundary conditions used for LES of combustion instabilities. There are many

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paths to use LES to predict unstable combustion in a burner. Two strategies are usually utilized:

(1) Forced modes: the first method is to force the combustor using predetermined forcing strategies (for example, exciting the velocity field at the inlet of the burner) and measuring the response of the burner (for example, the time delay between flow rate oscillations and unsteady reaction rate). Such information is a building block of acoustic models which try to predict the behavior of the combustor by decomposing it into acoustic elements (McManus *et al.* 1993). The burner itself is one such part, and LES is used to determine its transfer function. The actual existence and characteristic of combustion modes are then determined by the acoustic code (generally a one-dimensional code).

(2) Self-excited modes: a second and more ambitious method is to compute with LES the entire combustor geometry, including inlets and outlets, far enough to stop at places where well-defined acoustic boundary conditions can be defined. Then, the LES code should exhibit self-excited modes (limit cycles) exactly like the real experiment, providing the right frequency but also the mode amplitude.

Both strategies have advantages and drawbacks as listed below:

FORCED MODES

- A prerequisite condition for forcing is that a relatively ‘stable’ baseline regime is attained upon which forcing is subsequently applied. If the computed combustion regime is always unstable, this strategy cannot be used. In experiments, one method is to take flames out of the burner and let them burn in free space, thereby suppressing most possible acoustic coupling modes. Computationally this is not the way to go as ‘free space’ computations are even more demanding in terms of specifying and implementing boundary conditions.
- Forced modes are rather fast to compute because the computational domain is smaller and less cycles are required to obtain the forced response.
- Forced modes cannot predict transverse acoustic modes since those are not introduced by inlets, but are created inside the chamber itself.
- Forced modes can be easily used to measure the reflection coefficients of combustion chambers as done experimentally by Poinsot *et al.* (1986).

SELF-EXCITED MODES

- The first advantage of self-excited computations is that they are similar to experiments; they will capture any mode as long as it gets amplified. Transverse modes, for example, will naturally be captured.
- Self-excited modes may require long computing times due to the large computational domain; limit cycles may require many periods to be reached. Many combustors exhibit hysteresis phenomena and a long transition time from stable to unstable operation. Having to wait a few seconds for a burner to reach a steady and reproducible limit-cycle in an experiment is common. Computing the thousands of cycles associated to such a transition is out of question for LES methods.
- Self-excited modes computations rely heavily on the precision of all sub-models and of proper boundary conditions; if one boundary condition is not accurately

prescribed, no limit cycle or the wrong limit cycle will be obtained. Considering the high costs of such computations, this is a major drawback.

- Self-excited modes may depend on initial conditions. Many combustors are non linearly unstable, meaning that some initial perturbation must be brought to the flow to start oscillating. Determining numerically which type of initial condition is adequate for testing stability is a difficult task.

Successful computations of both self-excited (Kailasanath *et al.* 1985, 1991) and forced modes (Angelberger *et al.* 1998) may be found in the literature, indicating that either strategy may be valid. However, depending on the exact geometry of the burner, one technique usually proves superior over the other.

2. Configuration and scope of present study

For the present study we investigated the effects of initial and boundary conditions for LES computations of a gas turbine burner. The geometry of the combustor is displayed in Fig. 1.

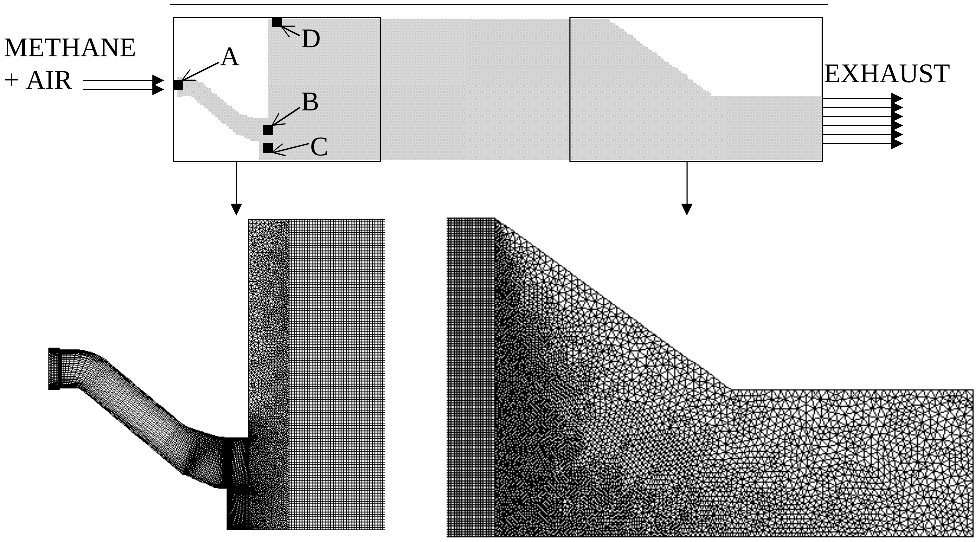

FIGURE 1. Burner geometry and unstructured mesh

For this geometry, different initial and boundary conditions were tested for LES. The objectives were to investigate (1) the time required for the flow to reach equilibrium, (2) the existence of a 'stable' regime on which forcing could be used and (3) the existence of self-excited modes and the capacity of the code to predict limit cycles.

3. Chemistry and flame/turbulence LES model

Premixed methane-air is injected into a dump combustion chamber terminated by a convergent section. For the present study, the inlet pressure and temperature are 1 bar and 300 K respectively. The chemistry is obtained by the ICC procedure; a single-step reaction $CH_4 + O_2 \rightarrow CO_2 + 2H_2O$ is used. The flame speed is 23 cm/s and the adiabatic flame temperature 1820 K. The structure of the laminar unthickened flame is displayed in Fig. 2 and compared to the solution provided by PREMIX using adaptive meshes and a steady solution algorithm. The flame thickness computed using the maximum temperature gradient is 0.6 mm.

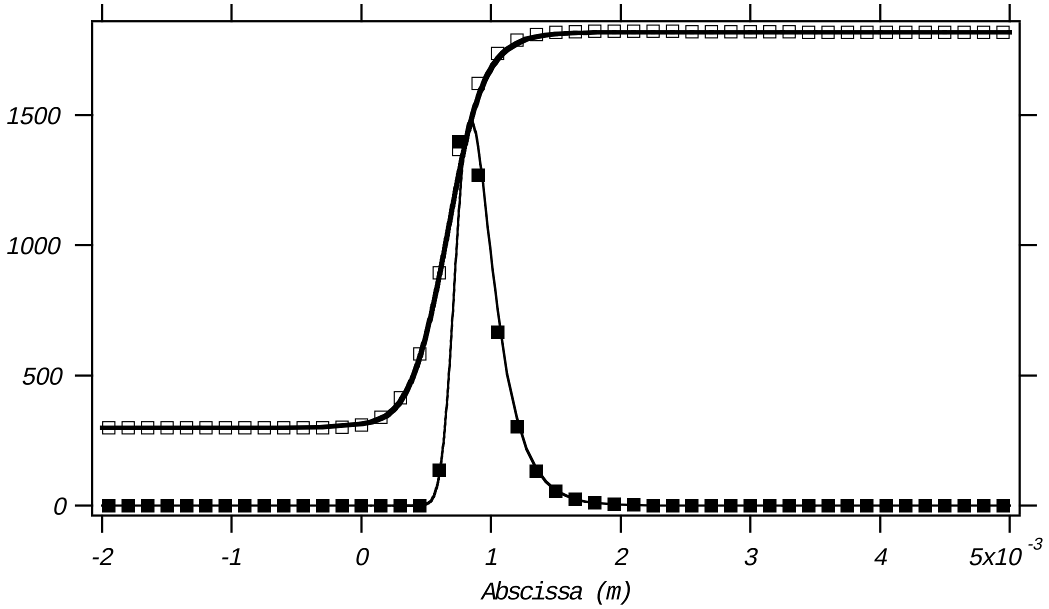

FIGURE 2. Structure of the premixed methane/air flame. Comparison with PREMIX. Temperature: AVBP (□), PREMIX (——). Reaction rate for energy (/10^6): AVBP (■), PREMIX (——).

The interaction between turbulence and flame is modeled using the thickened flame approach developed at CTR in 1997 and 1998 (Veynante and Poinsot 1997, Angelberger *et al.* 1998). The thickening factor is 30. To account for subgrid scale wrinkling effects, the efficiency function of Colin *et al.* (1999) is applied.

4. Boundary and initial conditions

Boundary conditions raise specific questions for combustion instabilities. Inlet conditions must impose a subsonic mean flow rate, but they must, at the same time, be non-reflecting for acoustic waves leaving the domain if resonance is to be avoided. In the same way, outlet conditions must be non-reflecting but must maintain a fixed level of mean pressure (1 atm in the present case). In AVBP, these constraints are satisfied by using an evolution of the NSCBC method (Poinsot and Lele 1992) in which waves entering the domain at the inlet are written:

$$\mathcal{L} = \sigma(U(x,y,z,t) - U_{in}(x,y,z))$$

where $U_{in}(x,y,z)$ is the 'target' mean velocity profile and σ is a relaxation constant. Large values of σ provide a strong control of the inlet velocity and a reflection coefficient which can be quite high while smaller values of σ let the inlet velocities fluctuate around their target values when acoustic waves propagate upstream, leading to an (almost) non-reflecting boundary.

At the outlet, both non-reflecting and reflecting conditions ($p' = 0$) were tested.

Initial conditions correspond to a jet of fresh gases entering the chamber which is filled with burnt gases. The flow is then left to evolve in time.

5. Reacting flow with non-reflecting inlet and outlet

The first test case corresponds to a non-reflecting outlet. The objective was to create a 'stable' flow on which perturbations could be added to study the forced response of the burner. This proved to be impossible. As soon as the flow starts to establish, a strong self-excited oscillation develops. The computation was run for a total time of 0.1 ms, corresponding to more than 50 acoustic cycles, and no damping of this mode was observed. A limit cycle is rapidly observed at a frequency of 520 Hz. Figs. 3 and 4 show the evolution of the inlet pressure and velocity measured at point A.

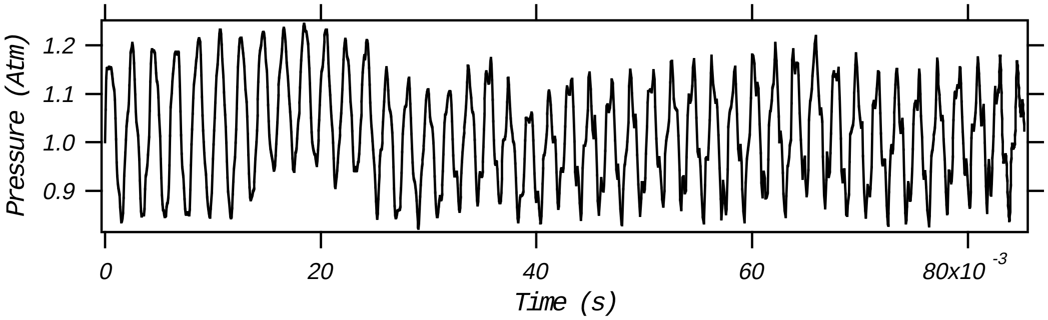

FIGURE 3. Time evolution of inlet pressure (Point A) for a non-reflecting outlet configuration.

The 'soft' inlet condition tries to maintain the inlet velocity close to the target value (of the order of 34 m/s), but the waves propagating upstream from the chamber affect the inlet velocity significantly. The overall pressure oscillation in the inlet is very large: of the order of 0.15 atm. In the combustion chamber, lower amplitudes are exhibited: typically less than 0.1 atm.

Instantaneous fields of fuel mass fraction at three instants are displayed in Fig. 5. The wrinkling of the flame (even when thickened) is very high, and combustion takes place over a small region. All the fresh gas burns within the combustion chamber. The existence of pockets of fresh gases which are shed from the main reactant stream and burn while they convect downstream is characteristic of combustion instabilities.

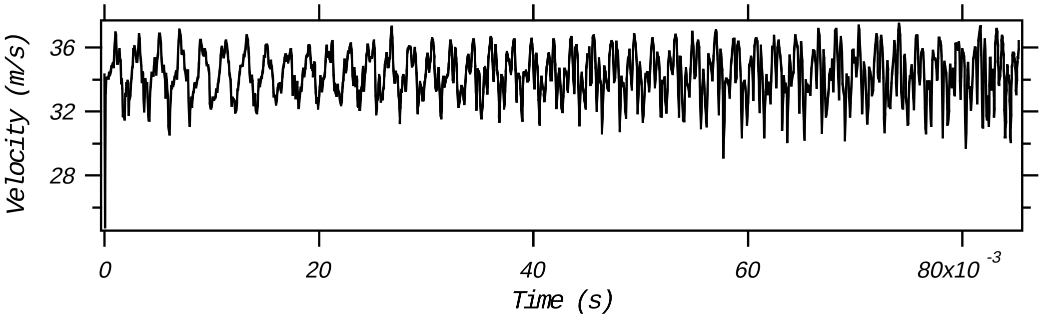

FIGURE 4. Time evolution of inlet velocity (Point A) for a non-reflecting outlet configuration.

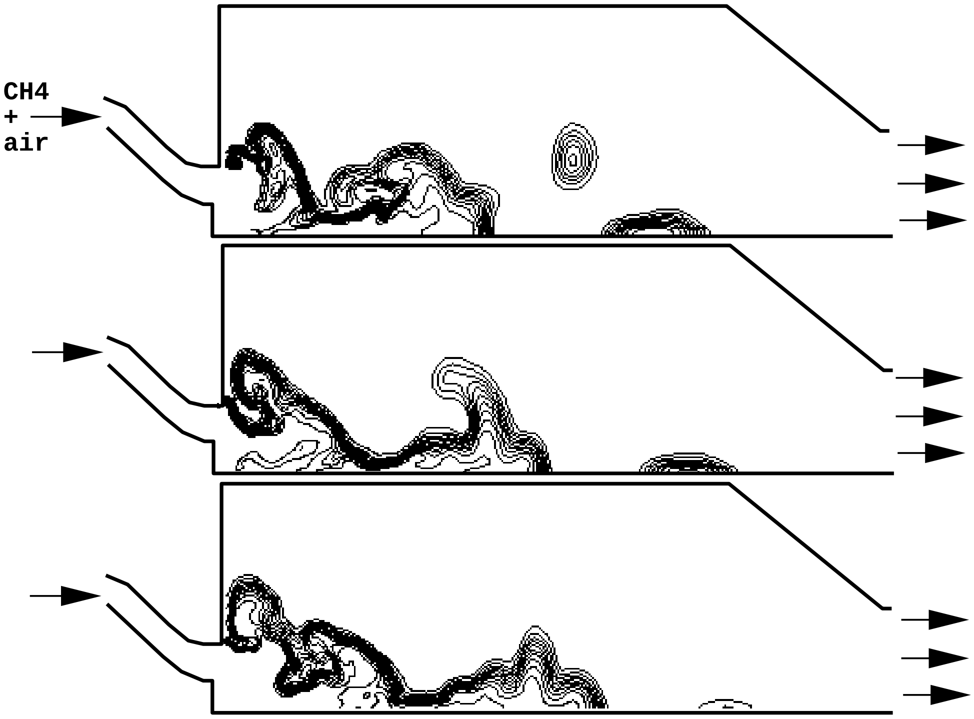

FIGURE 5. Fields of fuel mass fraction at three instants during one limit cycle for a configuration with non-reflecting outlet.

The flame is stabilized at the dump but oscillates strongly. A significant part of this movement is due to the intense acoustic field found at the entrance of the dump. Inside the chamber, in addition to the 520 Hz mode evidenced at the inlet of of the intake duct, transverse mode oscillations are observed at a frequency of 1800 Hz. The velocity perturbations induced by such strong acoustic fluctuations are large; they scale with $p'/(\rho c)$ and can reach 10 m/s for transverse oscillations and 20 m/s inside the intake duct. This has two consequences:

- The velocity modulation in the intake duct drives the flame motions; the distance between two burning vortices in Fig. 5 corresponds to the wavelength induced by the 520 Hz modulation on the incoming jet at 34 m/s. More importantly, the velocities induced by the acoustic perturbations are of the order of the mean flow velocity, suggesting that the velocity in the intake could change sign if the oscillations become strong, thereby leading to flashback (see next section).

- The transverse velocity perturbations also influence flame wrinkling, and the smallest wavelengths observed for the flame perturbations correspond to acoustic perturbations. Acoustic velocities at the dump section create flame deformations which are then convected downstream. The existence of a transverse mode is confirmed by pressure traces at points C (lower wall) and D (upper wall) displayed in Fig. 6. These points oscillate with opposite phases. The corresponding frequency (1800 Hz) matches the first transverse frequency of the burner. The corresponding mode has a velocity anti node located in the middle of the chamber, where the flame develops.

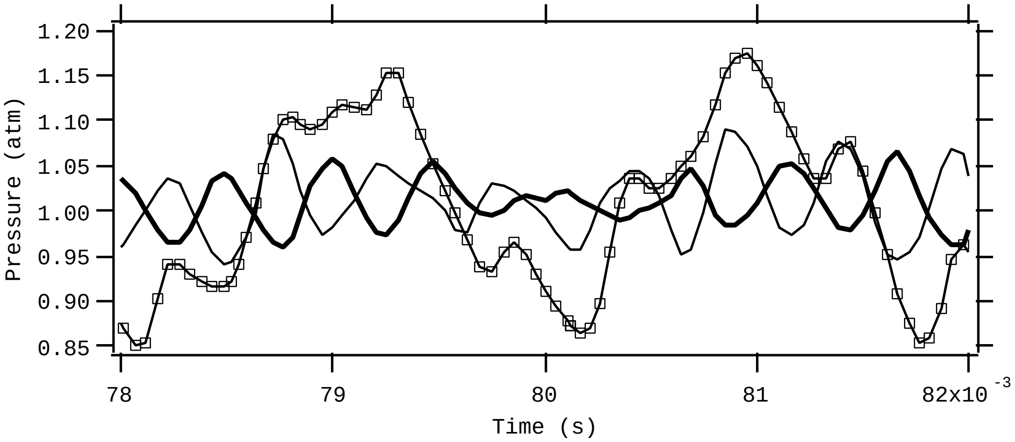

FIGURE 6. Pressure traces at points D (upper wall, ━━), C (lower wall, ——) and A (inlet, □)

6. Reacting flow with reflecting outlet

Since it was impossible to obtain a stable baseline flow suited to the application of forcing, self-sustained oscillations were studied. The previous case (with non-reflecting outlet) is actually a self-sustained instability, but a more realistic case is a combustion chamber ending in a large vessel or in open atmosphere like in many laboratory experiments. In this case, the outlet is reflecting and the condition corresponding to such outlets is that pressure is imposed. This was done here by continuing the previous computation after $t = 85$ms but fixing the outlet pressure to 1 bar. Nothing else was changed.

Figure 7 shows the evolution of the inlet pressure; as soon as the outlet pressure is fixed, acoustic waves cannot leave the domain through the outlet and are reflected. The instability increases, and the oscillation amplitude grows. The oscillation is strong enough to induce backflow in the air intake duct, and the flame is able to flashback into the intake duct. Such behavior is observed experimentally (Keller *et al.* 1981) and usually leads to considerable damage for the installation. Figure 8 shows fields of fuel mass fraction during one cycle of oscillation of Fig. 7. Fig. 9

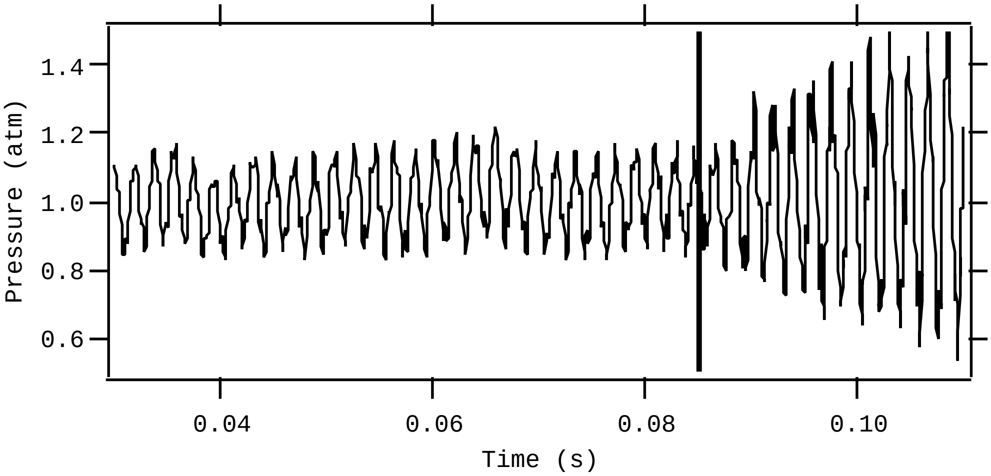

FIGURE 7. Evolution of inlet pressure (Point A). Before $t = 0.85$ ms, non-reflecting conditions are used at the outlet. After $t < 0.85$ ms, pressure is fixed.

displays the instants used in Fig. 7 on the time evolution of a longitudinal velocity at point B located at the dump section (Fig. 1).

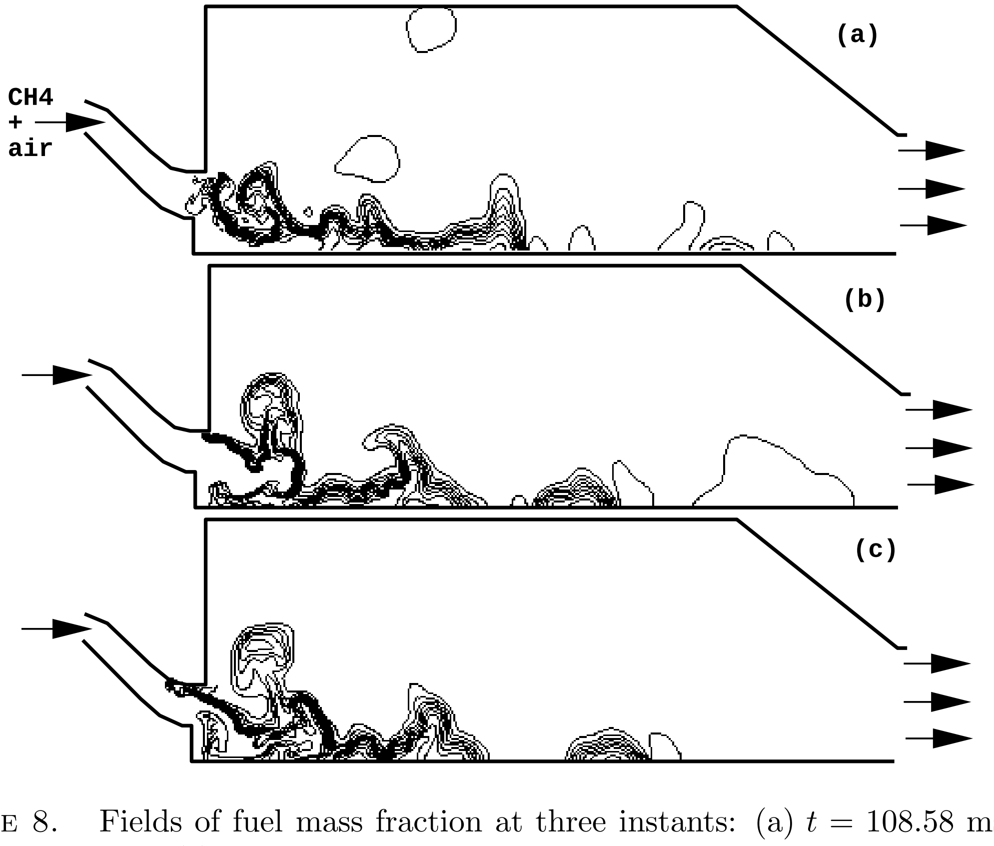

FIGURE 8. Fields of fuel mass fraction at three instants: (a) $t = 108.58$ ms (b) $t = 109.56$ ms and (c) $t = 109.99$ ms.

In Fig. 8a, the flame is first pushed out of the intake duct inside the combustion chamber. The velocity at the dump is increasing at this instant (Fig. 9) and keeps increasing until t = 0.109 ms. This velocity surge creates a vortex containing fresh fuel and additional flame surface as seen in Fig 8b. In the second half of the instability cycle, the velocity at the injection plane decreases and may become negative. At this point (Figs. 8b and c), the flame flashes back into the intake duct. This flashback is observed both in the upper and lower part of the intake duct; there, the recirculation zone which contained fresh gases gets filled by burnt gases which reach the intake duct but cannot enter it because the velocity field is already increasing again.

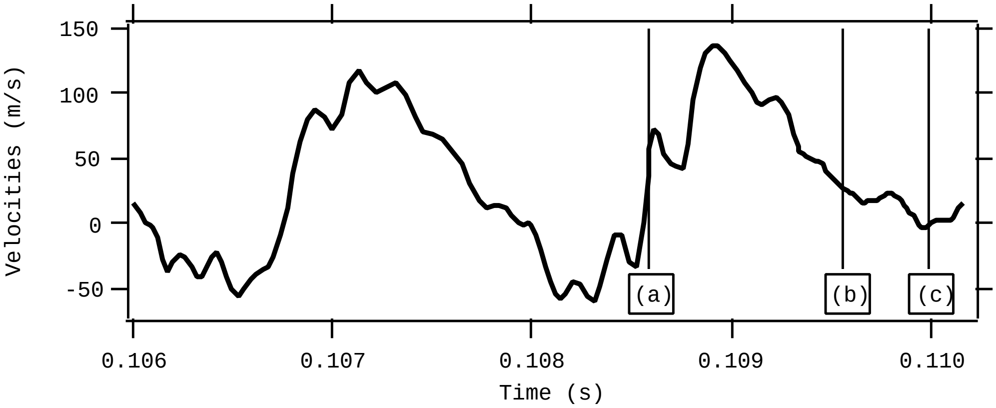

FIGURE 9. Evolution of longitudinal velocity at the entrance of the dump. The three instants used for Fig. 8 are visualized by vertical lines.)

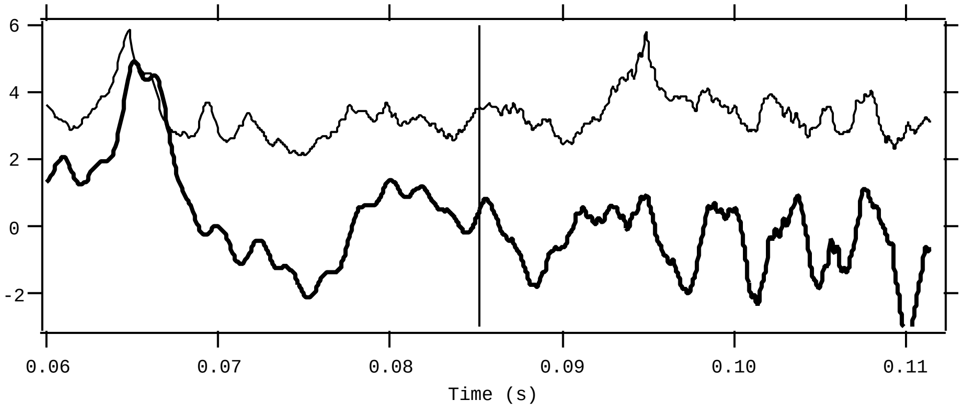

FIGURE 10. Variations of total reaction rate (———) and normalized average pressure in the combustor (━━━) for non-reflecting outlet (before $t = 85$ ms) and reflecting outlet (after $t = 85$ ms).

The vortex formation during the velocity surge (between instants (a) and (b) on Fig. 8) is the source of the instability; these pockets burn downstream and feed energy into the instability mode. This mechanism was already present for the non-reflecting outlet but never strong enough to induce flashback. Closing acoustically the outlet provides a stronger interaction as shown in Fig. 10; the total reaction rate and the mean pressure in the combustor follow similar evolutions before the outlet is acoustically closed (at $t = 85$ ms), but their correlation increases after the outlet becomes reflecting. After $t = 100$ ms the reaction rate starts oscillating in phase with pressure at 520 Hz, indicating a strong coupling between unsteady heat release and the acoustic field.

7. Conclusion

LES of confined turbulent premixed flames were performed to investigate the influence of initial and boundary conditions to explore possible investigation strategies for combustion instabilities. Of particular interest was the choice between tests where the chamber is forced externally and tests under a self-excited mode. It was found that, even for non-reflecting outlet conditions and 'soft' non-reflecting inlet conditions, a self-sustained combustion instability develops rapidly inside the chamber. A limit cycle of strong amplitude is reached, making studies of forced response impossible. Self-sustained oscillations studies are, therefore, the only possible strategy for this burner. The self-sustained oscillation mode appears to be very dependent on boundary conditions; when the outlet condition is changed from non-reflecting to a reflecting (imposed pressure) condition, the amplitude of the oscillation increases up to the point where the flame flashes back into the air intake of the burner.

8. Acknowledgments

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