LARGE EDDY SIMULATIONS OF COMBUSTION INSTABILITIES

Thierry Poinsot
IMF Toulouse and CERFACS, Toulouse France
Christian Angelberger
CERFACS, Toulouse France
Fokion Egolfopoulos
University of Southern California, USA
Denis Veynante
Laboratoire EM2C, CNRS and Ecole Centrale Paris, France

ABSTRACT

This paper describes a Large Eddy Simulation of acoustic combustion instabilities in a dump combustor. It is shown that the main effect of acoustic waves entering the combustion chamber is to create large vortices and unsteady heat release when these vortices burn. The fact that the equivalence ratio of incoming gas is also modulated by acoustic waves was tested through a special simulation where the inlet equivalence ratio fluctuates but the total flow rate remains constant. This mechanism was shown to induce less destabilizing effects than the purely aerodynamical mechanism due to vortex formation and combustion.

MOTIVATIONS AND OBJECTIVES

Computing unsteady reacting flows accurately can not always be achieved using classical Reynolds Averaged Navier Stokes (RANS) approaches. Turbulent combustion phenomena such as flame flashback, blowoff or combustion instabilities (McManus et al 1993, Poinsot and Candel 1988, Candel et al 1996) are not well defined in a RANS framework where only time- averaged quantities are solved for. For such problems, where the intrinsically unsteady nature of the flow makes RANS clearly inadequate. large eddy simulation (LES) techniques are viewed today as a promising tool.

Interestingly, LES may be easier to perform in unsteady flames than in steady turbulent flames: flows submitted to instabilities are dominated and controlled by very large eddies and, accordingly, it is likely that a limited range of eddies has to be incorporated to describe the interaction between turbulence and chemistry in such flows (Bray et al 1989, Baum et al 1994).

This paper describes a LES study of combustion instabilities in a laboratory burner. More specifically, we use LES to address a question of interest for modern lean combustors: to satisfy emission regulations, modern gas turbines operate in very lean combustion regimes. These flames are extremely sensitive to combustion oscillations but the exact phenomena leading to instabilities are still discussed. A central question for modeling approaches is to determine the phenomena inducing unsteady reaction rates, required to sustain oscillations, when an acoustic wave enters the combustion chamber. This may be due (at least) to two main effects:

- the formation of vortices in the combustion chamber. These vortices capture a large pocket of fresh gases which burns only at later times in a violent process leading to small scale turbulence and high reaction rates.
- a modification of the fuel and oxidizer flow rates when the acoustic wave propagates into the fuel and air feeding lines. This will lead to a change of the equivalence ratio and therefore to a modification of the burning rate when these pockets enter the chamber. If the burner operates in a very lean mode, this effect may be important since a non-flamable mixture may enter the combustion zone.

The objective of the present work is to examine, using LES, which mechanism is predominant in the case of a backward facing step premixed burner developed at Ecole Centrale Paris (ECP). An extensive set of experimental results is available for this burner (Poinsot et al 1986, 1987, 1988) and this configuration is also similar to many classical combustion instabilities experiments (see for example Keller et al 1981) and multiple industrial devices. To achieve this objective, multiple tools were integrated:

• A LES solver able to handle complex geometries. Multiple techniques have been proposed in the past to perform LES of turbulent premixed combustion (Menon and Kerstein 1992, Bourlioux et al 1996, Smith and Menon 1996, 1997, Im et al 1996, Piana et al 1996, 1997, Veynante and Poinsot 1997a,b). Few of them have been used in a realistic configuration (see for example Kailasanath et al 1985, 1991 or Veynante and Poinsot 1997b). Real combustion chambers will require meshes able to deal with highly complex geometries. For the present work, we used an hybrid mesh code called AVBP and developed at CERFACS on top of a parallel library COUPL produced jointly by CERFACS and Oxford University. AVBP has been used for a variety of unsteady flows using DNS and LES (Nicoud et al 1996, Nicoud 1997, Ducros et al 1997).

• The choice of a proper chemical description remains a critical issue in all reacting flows. In the present study, a new technique called ICC (Integrated Complex Chemistry) is used to construct reduced chemical schemes able to predict changes in equivalence ratio for methane and propane. This methodology follows the usual approach of heuristic scheme reduction (Westbrook and Dryer 1981) and will not be described here. A complete description of ICC may be found in (Bedat et al 1997, 1999).

• Thermal boundary conditions at the walls of the combustion chamber control flame stabilization and quenching (Veynante and Poinsot 1997b). These conditions are sometimes unknown. For the present study, where the configuration corresponds to a burner developed at Ecole Centrale and built with ceramic plates, walls are assumed to be adiabatic (Poinsot et al 1987).

• to describe flame - turbulence interactions in the LES, we used the Thickened Flame (TF) approach initially proposed by O'Rourke and Bracco (1979). The flame thickening approach requires subgrid scale wrinkling models obtained from direct numerical simulations of flame vortex interactions for various flame thickening factors (Veynante and Poinsot 1997b, Angelberger et al 1998).

CONFIGURATION

The configuration studied here is displayed on Fig. 1. An acoustic wave traveling along the air feeding line of a backward facing step combustor introduces an air flow rate perturbation $\dot{m}_a'$ of the mean air flow rate $\dot{m}_a$. The mean equivalence ratio is ϕ. When the acoustic wave passes near the gas injection system, a fluctuation of the fuel flow rate $\dot{m}_f'$ is created. The perturbation of the equivalence ratio ϕ' due to the acoustic wave is given by: $\frac{\phi'}{\phi} = \frac{\dot{m}_f'}{\dot{m}_f} - \frac{\dot{m}_a'}{\dot{m}_a}$

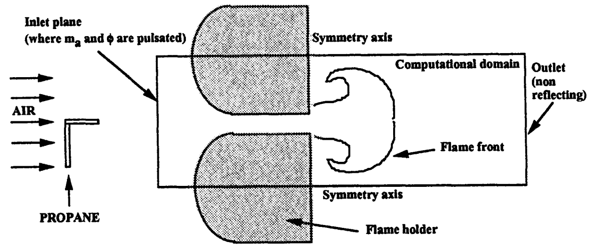

Figure 1: Configuration for simulations of combustion instabilities: the propane - air burner used by Poinsot et al (1987). Only one of the injection slots is computed (the real system had five slots). The computational domain is 22.4 cm long and 2 cm high.

This perturbation of the equivalence ratio will influence the burning rate. But the hydrodynamic effect of $\dot{m}_a'$ is also to induce the formation of a vortex near the chamber dump. These two effects may be isolated by performing the following simulations:

• Case A ($\phi' = 0$): Aerodynamical (or acoustic) forcing of the chamber. In this case the inlet flow rate fluctuates but the equivalence ratio remains constant. This may be achieved for example by assuming that the distance between the fuel injector and the chamber is very long or assuming that both fuel and air lines react in the same way to acoustic perturbations (i.e. $\dot{m}_f'/\dot{m}_f = \dot{m}_a'/\dot{m}_a$).

• Case C (total flow rate is constant): Chemical forcing of the chamber (modulation of inlet equivalence ratio). The effects of equivalence ratio changes are isolated assuming that a change of $\dot{m}_a$ induces *only* a change in equivalence ratio. The total flow rate is assumed to remain constant so that no hydrodynamic forcing may occur: only chemical effects are kept in the simulation. Obviously the real situation corresponds to a case where chemical and acoustic forcing are combined.

REDUCED CHEMISTRY FOR LES

Our objectives require to compute flames with variable equivalence ratio and an important task is to derive a simplified kinetic scheme which would closely predict several global flame properties. This was done for lean methane / air and propane / air mixtures for pressure $P = 1$ atm and fresh gases temperature $T_0 = 300$ K, corresponding to the operating conditions of the Ecole Centrale experiment.

The development of a simplified scheme was obtained through the ICC technique (Mantel et al 1996; Bedat et al 1997, Angelberger et al 1999). Traditionally, simplified schemes, such as one-step chemistry, have been derived by simply matching laminar flame speeds and such schemes have been extensively used in simulations of turbulent reacting flows. The ICC technique adds to laminar flame speeds the prediction of strain rate effects and the description of flame structure using simple chemical schemes. This is an important advantage because reacting fronts can be subjected to a large range of strain rates in multi-dimensional, high-Reynolds-number simulations. In the previous ICC studies (Mantel et al , 1996; Bedat et al , 1997) simplified chemical mechanisms were derived for a fixed equivalence ratio. In the present study the ICC technique was extended in order to account for variable equivalence ratio as well as for flame thickening imposed by the necessity to resolve the flame structure using an LES grid.

A one-step global chemistry model was derived, describing several flame properties of lean propane/air mixtures at $P = 1$ atm and $T_0 = 300$ K. The scheme is:

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

with the specific reaction rate given by: $\dot{\omega} = [C_3H_8]^a[O_2]^b A exp(-E_a/RT)$ where $[C_3H_8]$ and $[O_2]$ are the molar concentrations of the reactants, a and b the corresponding concentration exponents, A the pre-exponential factor, E_a the activation energy, R the gas constant, and T the absolute local gas temperature. After comparison with the full chemistry results, the following parameters were kept for propane: $a = 1.0$, $b = 0.5$, $A = 1.60E09$ (cgs units), $E_a = 14,000$ (cal/mole).

Fig. 2 depicts the experimental (Vagelopoulos and Egolfopoulos, 1998) laminar flame speeds, s_l^0, for atmospheric, lean C_3H_8/air mixtures as well as the predictions obtained by using detailed chemical kinetics and transport and the proposed simplified scheme. The agreement is quite satisfactory. The detailed chemistry for C_3H_8 was compiled by combining a C3 sub-mechanism (Pitz and Westbrook, 1986) with the well-established C1-C2 GRI 2.1 mechanism (Bowman et al , 1996). Additional cases for strained flames were also computed and may be found in (Angelberger et al 1999).

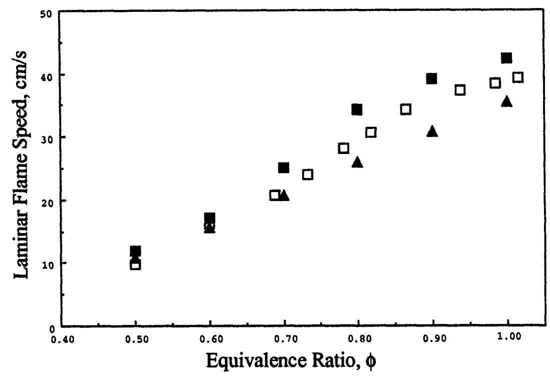

Figure 2: Variation of laminar flame speed with equivalence ratio for atmospheric C_3H_8/air mixtures with reactants at initial temperature $T_0 = 300$ K. squares: experiments; filled squares: detailed chemistry computations; triangles: ICC computations.

LES WITHOUT FORCING

Simulations were first performed for the unforced flow in the ECP burner. The previous models for chemistry and flame turbulence interaction were incorporated into this code and tested separately. The operating point corresponds to an inlet temperature of 300 K, an equivalence ratio of 1, an inlet velocity of 6.4 m/s. The flame speed is 0.36 m/s and the adiabatic flame temperature 2190 K.

All computations were performed in two dimensions since flow vizualisations have indicated that large scale structures produced in this chamber were indeed two-dimensional (this was one of the objectives of this design). A grid of 41000 points was used. The filtered Smagorinski model was used for the dynamic field. For all cases, the combustion chamber is computed as an amplifier system (and not as a resonator): inlet and outlet boundary conditions are non reflecting and all acoustic waves produced in the combustor are allowed to leave the chamber so that no self-induced low-frequency mode can occur. The combustor can then be forced to study its response. Forcing is introduced at the inlet of the combustor by modulating the incoming acoustic wave or the incoming gas equivalence ratio following the NSCBC technique (Poinsot and Lele 1992).

Typical simulations run during 500000 iterations, corresponding to 100 acoustic travel times in the chamber and more than 4 convective times. Initialization of computations in such cases is not simple since the LES code has low levels of dissipation: the computation starts from an initial state where a strip of fresh gas is located in the combustion chamber and surrounded by

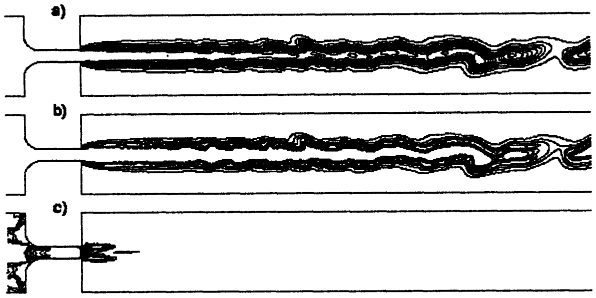

Figure 3: Instantaneous fields of temperature (a), reaction rate (b) and subgrid scale turbulent velocity (c) for an unforced regime.

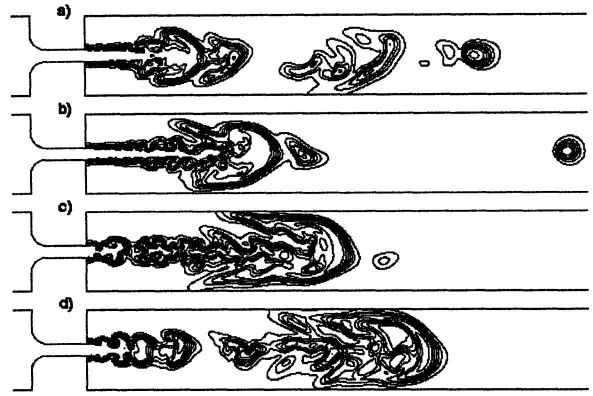

Figure 4: Temperature fields during one forcing cycle at 530 Hz. Time separation between each picture: a quarter period (0.47 ms)

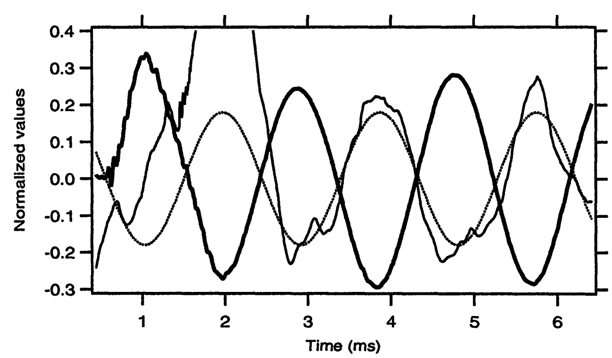

Figure 5: Time evolutions of inlet flow rate (thick line), window-integrated reaction rate in the LES (solid) and in the experiment (dashed).

two strips of burnt gas on each side. To allow stabilization during this first phase, artificial viscosity (fourth-order) is used. After a few transit times in the burner, artificial viscosity is suppressed.

A typical snapshot of the flow for this regime is given in Fig. 3. The flame is only slightly corrugated and corresponds to the state observed in the experimental set-up in the absence of instabilities (Fig. 6 in Poinsot et al 1987).

Forced response of the Ecole Centrale burner

The first excitation case corresponds directly to the experiment of Poinsot et al (1987): the objective is to reproduce the combustor response to a 530 Hz excitation of the inlet flow rate corresponding to one of the strongest instability modes observed in the chamber. More precisely, LES is used to measure the time delay between inlet flow rate perturbations and reaction rate oscillations. This delay was measured in the experiment and found to be close to 0.9 ms (Fig. 12 in Poinsot et al 1987). The wave amplitude is chosen to induce a flow rate change equal to 50 percent of the mean flow rate. The forcing frequency is 530 Hz.

Snapshots of temperature during one cycle of forcing are displayed on Figs. 4. The general features observed in the LES match those observed in the experiment: a large mushroom-shaped structure is produced (similar to vortices observed in impulsively-started jets) and leads to a high increase of flame surface and reaction rate. Fig. 5 displays time variations of inlet flow rate and heat release. The reaction rate lags the inlet flow rate by approximately 0.9 ms as seen in the experiment. The experimental heat release measured (using phase averaging by Poinsot and co workers) is also displayed and a very good agreement on phases is obtained.

In a second stage, the combustor was forced by modulating the inlet equivalence ratio ϕ between 0.3 and 1.7 using a sinusoidal function at the same frequency of 530 Hz. The amplitude chosen for this modulation is large to maximize its effects. To achieve such levels, both fuel and air flow rates would have to be affected by the acoustic wave and in opposite directions: the fuel flow rate should decrease when the air flow rate increases. Since this is unlikely to happen in practice, the present simulations provide a maximization of potential effects of unmixedness on combustor response. The overall mass flow rate was kept constant so that no vortices were formed at the inlet and only the chemistry effect was active at least during the initiation of the oscillations. Fig. 6 shows how the lean and rich regions created at the inlet enter the combustor and affect the flame front.

Finally, Fig. 7 compares the effects of acoustic forcing (case A) with those of chemical forcing (Case C). The

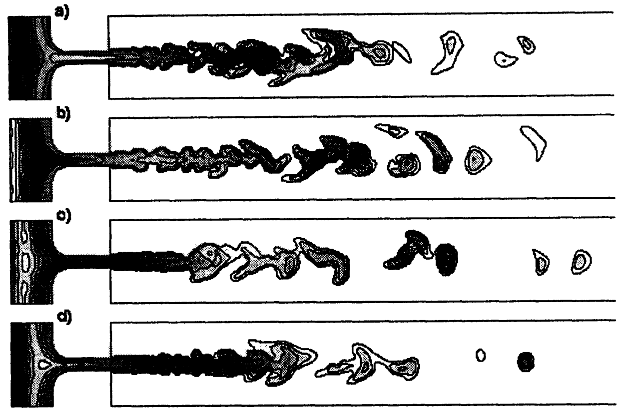

Figure 6: Fuel mass fraction fields during one forcing cycle at 530 Hz (modulation of equivalence ratio ϕ).

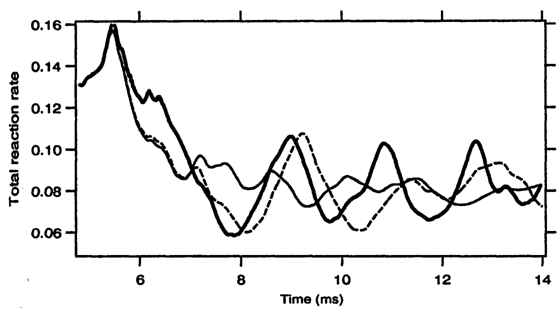

Figure 7: Total reaction rate vs time for unforced flow (solid line), acoustic forcing at 530 Hz with an amplitude of 50 percent (thick line) and for a modulation of equivalence ratio between 0.3 and 1.7 (dashed line).

case without forcing is added for reference. Obviously, runs should be continued to confirm this analysis but it appears that acoustic forcing has a stronger effect on the total reaction rate than chemical forcing. Since we chose a very large range of variations for the chemical forcing, it seems that acoustic forcing is the main phenomenon to consider for combustion instabilities in the present system.

Conclusion

Large eddy simulations of the effects of acoustic waves and equivalence ratio variations on flame response have been performed for a premixed turbulent flame stabilized in a backward-facing step combustor. The developed code includes (1) a chemistry model based on a new reduction technique called ICC for propane and methane (2) a flame thickening methodology to handle flame turbulence interactions and (3) specific boundary conditions to control and measure acoustic wave reflections on inlets and outlets. The chemistry reduction method (called ICC) was derived and validated by comparing its result with full schemes / full transport results obtained with stagnation point flame codes. The code itself is a compressible parallel finite volume solver able to handle hybrid grids (AVBP).

Results indicate that the final tool was able to predict forced combustor response over many excitation cycles and to reproduce the phenomena observed in the experiment of Ecole Centrale Paris. The phase between flow rate oscillations and unsteady heat release, for example, was recovered in the case of acoustic forcing.

Modulating the inlet equivalence ratio also lead to unsteady heat release but with lower amplitudes than with acoustic forcing.

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