Compressible Large Eddy Simulation of turbulent combustion in complex geometry on unstructured meshes

L. Selle\textsuperscript{a}, G. Lartigue\textsuperscript{a}, T. Poinsot\textsuperscript{b}, R. Koch\textsuperscript{c}, K.-U. Schildmacher\textsuperscript{c}, W. Krebs\textsuperscript{d}, P. Kaufmann\textsuperscript{d} and D. Veynante\textsuperscript{e}

\textsuperscript{a}CERFACS, CFD team, 42 Av. G. Coriolis, 31057 Toulouse Cedex, France
\textsuperscript{b}IMF Toulouse, UMR CNRS/INP-UPS 5502, Allée du Pr. C. Soula, 31400 Toulouse CEDEX, France
\textsuperscript{c}Institute of Thermal Turbomachinery, University of Karlsruhe, Kaiserstrasse 12, 76128 Karlsruhe, Germany
\textsuperscript{d}Siemens PG, Mullheim, Germany
\textsuperscript{e}Laboratoire EM2C, Ecole Centrale de Paris and CNRS, 92295 Châtenay Malabry CEDEX, France

Abstract

Large Eddy Simulations of an industrial gas turbine burner are performed for both non-reacting and reacting flow using a compressible unstructured solver. Results are compared to experimental data in terms of axial and azimuthal velocities (mean and RMS), averaged temperature and existence of natural instabilities such as PVC (precessing vortex core). The LES is performed with a reduced two-step mechanism for methane - air combustion and a Thickened Flame model. The regime of combustion is fully premixed and the computation includes part of the swirler vanes. For this very complex geometry, results demonstrate the capacity of the LES to predict the mean flow, with and without combustion as well as its main unstable modes: it is shown for example that the PVC mode is very strong for the cold flow but disappears with combustion.

Key words: Large-Eddy Simulation, Combustion, Acoustics, Complex geometries

1 INTRODUCTION

Large Eddy Simulation (LES) are becoming standard tools to study the dynamics of turbulent flames (see for example recent Summer Programs at CTR, special issue
of *Flow Turbulence and Combustion* (65, 2000) on LES of reacting flows or recent books on turbulent combustion [1, 2]. Multiple recent papers have demonstrated the power of these methods [3 – 9]. For example, LES appears as one of the key tools to predict and study combustion instabilities encountered in many modern combustion devices such as aero or industrial gas turbines, rocket engines or industrial furnaces.

Up to now, most LES of reacting flows have been limited to fairly simple geometries for obvious reasons of cost and complexity reduction. In many cases, experiments have been designed using especially simple shapes (two-dimensional [3, 7, 10] or axisymmetrical configurations [11, 12]) and simple regimes (low speed fbws, fully premixed or fully non-premixed flames) to allow research to focus on the physics of the LES (subgrid scale models, flame / turbulence interaction model) and more generally to demonstrate the validity of the LES concept in academic cases. Even though this approach is clearly adequate in terms of model development, it is important to recognize that it can also be misleading in various aspects when it comes to deal with complex flames in complex geometries:

- Most LES of reacting flows have been performed in combustion chambers where structured meshes were sufficient to describe the geometry. In such solvers, using high-order spatial schemes (typically 4th to 6th order in space) is relatively easy and provides very precise numerical methods. As soon as real complex geometries are considered, these structured meshes must be replaced by unstructured grids on which constructing high-order schemes is a much more difficult task.
- Moving from structured to unstructured meshes also raises a variety of new problems in terms of subgrid scale filtering: defining filter sizes on a highly anisotropic irregular grid is another open research issue [13 – 16]). Many LES models, developed and tuned on regular hexahedral grids, will perform much more poorly on the poor-quality unstructured grids required to mesh real combustion chambers.
- Many laboratory flames used for LES validations are low-speed unconfined flames in which acoustics do not play a role and the Mach number remains small so that compressibility effects can be omitted from the equations ("low-Mach number approximation"). In most real flames (for example in gas turbines), however, compressibility can not be neglected: (1) the Mach number can reach much higher values and (2) acoustics are important so that taking into account compressibility effects becomes mandatory. This leads to a significantly heavier computational task: the time step becomes smaller and the boundary conditions must handle acoustic wave reflections [2]. Being able to preserve computational speed on a large number of processors then also becomes an issue simply to obtain a result in a finite time.
- In many combustion chambers, it is impossible to perform a true LES everywhere in the fbw. For example, the fbw between vanes in swirled burners or inside the ducts feeding dilution jets would require too many grid points. Multi-perforated plates which can create thousands of small jets cooling the combustion chamber, are also obviously beyond the present capacities of LES codes. As
a consequence, compromises must be sought and the LES of today and probably tomorrow require methods which offer (at least) robustness in places where the grid is not sufficient to resolve the unsteady flow. For such methods, having an excellent LES efficiency on high-quality grids for academic problems is not the most important issue anymore.

These few examples suggest that, when it comes to computing flames in complex geometries for real combustors, work must concentrate on new issues: unstructured solvers, compressible flows, boundary conditions, robustness in poorly meshed zones, parallel efficiency. This also means that many modeling aspects which were critical in simple laboratory flames (subgrid scale LES model for momentum, kinetic energy conservation, accuracy of chemistry description, etc) must now be combined with other (and sometimes more) critical problems: efficient unstructured solvers, subgrid scale LES models on “dirty” grids, boundary conditions adapted to acoustics…

The choice of a chemistry description is another difficulty. For most laboratory flames, describing chemistry with only one variable is sufficient for LES: the progress variable is enough to compute fully premixed flames and the mixture fraction is adequate for perfectly non-premixed piloted flames such as the Sandia flames (Combustion Research Facility division at Sandia: http://www.ca.sandia.gov/crf/index.html). In real gas turbines, however, the combustion regime is much more complex and more “robust” models are required to handle flames which are typically partially premixed with a full range of local equivalence ratios and mixing levels.

This study presents a computation of a complex industrial burner, developed at Siemens Power Generation, using an unstructured LES compressible solver. The main objectives are to:

- extend an existing flame / interaction model (called the Thickened Flame model) to a two-step chemical scheme,
- investigate the capacities of LES in a realistic configuration and
- compare the LES results to experimental data obtained at University of Karlsruhe. This comparison is performed for one regime only for which detailed LES and experimental results are gathered. This regime corresponds to a premixed case at an equivalence ratio of $\phi = 0.5$ and an inlet temperature of 673 K. This regime does not exhibit large scale combustion instabilities.

The LES solver used for the study is presented first. The TF (Thickened Flame) model is then discussed. A two-step chemical mechanism incorporating CO as the main intermediate species was tuned for the conditions of the Siemens burner and tested first for premixed laminar flames. The configuration used for the Siemens burner installed in the Karlsruhe combustion chamber is described before presenting cold flow results. Finally, reacting flow solutions are presented. For both reacting and non-reacting cases, the presentation includes a comparison of the averaged
fields (mean and RMS velocities for all cases; temperature for the reacting case), a study of the precessing vortex core and an analysis of the unsteady pressure in the burner which would control the structure vibrations in the real device.

2 THE LES SOLVER

The LES solver AVBP (see www.cerfacs.fr/cfd/CFDWeb.html) solves the full compressible Navier Stokes equations on hybrid (structured and unstructured) grids. Subgrid stresses are described by the WALE model [17]. The flame / turbulence interaction is modeled by the Thickened Flame (TF) model [3, 5, 7, 18, 19]. The numerical scheme uses third-order spatial accuracy and third-order time accuracy [20]. Tests performed during this study have demonstrated that the third-order spatial accuracy of the solver is a key feature to obtain precise LES results on unstructured meshes. The AVBP version used here also handles variable heat capacities: species enthalpies are tabulated and the mean heat capacity is determined as a function of temperature and species mass fractions $Y_k$. Therefore, local quantities such as the mean molecular weight $W$ or the ratio of heat capacities $\gamma$ are not constant. This introduces significant additional complexities in the numerical method, especially near boundaries where classical characteristic methods such as NSCBC [21] must be replaced by a more complex technique [22]. The walls of the combustion chamber are treated as adiabatic walls (the real experiment uses ceramic walls). Both no-slip and law-of-the-wall formulations have been used on walls with very limited differences on the results. Typical runs are performed on grids of 2.5 millions elements on 64 processors.

3 THE THICKENED FLAME MODEL

For the present study, only fully premixed flames are considered. Multiple studies have concentrated on LES of diffusion flames [8, 23, 24] while premixed cases have received less attention [9, 25 – 27]. Indeed, infinitely fast chemistry assumptions constitute a useful path for LES of diffusion flames. Such assumptions cannot be used for premixed flames, however: modelling the interaction between flame and turbulence in premixed combustion systems requires to track the flame front position, leading to a problem which is more difficult to handle than most diffusion flames. The natural technique to track the flame would be to solve its inner structure but this is impossible on typical LES meshes because premixed flame fronts are too thin. Two methods can then be used to propagate turbulent flame fronts on LES meshes:

- bring the flame thickness to zero and propagate the flame front as a thin interface: this is the principle of the G-equation method [1, 9],
thicken the flame so that it can be resolved on the LES mesh while still propagating at the same speed as the unthickened flame: this is the principle of the TF (Thickened Flame) model [2, 5].

In the present work, the standard TF model developed by Colin et al. [5] is used: in this model, preexponential constants and transport coefficients are both modified to offer thicker reaction zones that can be resolved on LES meshes. The fundamental property justifying this approach has been put forward by Butler and O’Rourke [28] by considering the balance equation for the k-species mass fraction $Y_k$ in a one-dimensional flame of thermal thickness $\delta^0_L$ and speed $s^0_L$:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u Y_k}{\partial x} = \frac{\partial}{\partial x} \left( \rho D_k \frac{\partial Y_k}{\partial x} \right) + \omega_k (Y_j, T) \tag{1}$$

Modifying this equation to have:

$$\frac{\partial \rho Y^{th}_k}{\partial t} + \frac{\partial \rho u Y^{th}_k}{\partial x} = \frac{\partial}{\partial x} \left( \rho FD_k \frac{\partial Y^{th}_k}{\partial x} \right) + \frac{1}{F} \omega_k (Y_j^t, T^t) \tag{2}$$

leads to a “thickened” flame equation where $F$ is the thickening factor and exponent $t^h$ stands for thickened quantities. Introducing the variable changes $X = x/F$; $\Theta = t/F$ leads to:

$$\frac{\partial \rho Y^{th}_k}{\partial \Theta} + \frac{\partial \rho u Y^{th}_k}{\partial X} = \frac{\partial}{\partial X} \left( \rho D_k \frac{\partial Y^{th}_k}{\partial X} \right) + \omega_k (Y_j^t, T^t) \tag{3}$$

which has the same solution as Eq. (1) and propagates the flame front at the same speed $s^0_L$. However, $Y^{th}_k(x, t) = Y_k(x/F, t/F)$ showing that the flame is thickened by a factor $F$. The thickened flame thickness is $\delta^1_L = F \delta^0_L$. Choosing sufficiently large values of $F$ allows to obtain a thickened flame which can be resolved on the LES mesh. Typically, if $n$ is the number of mesh points within the flame front required by the solver and $\Delta x$ the mesh size, the resolved flame thickness $\delta^1_L$ is $n \Delta x$ so that $F$ must be $F = n \Delta x / \delta^0_L$. For the computation of most flames using the TF model, values of $F$ ranging from 5 to 50 are sufficient to resolve the flame front on meshes corresponding to present computer capabilities. In the framework of LES, this approach has multiple advantages: when the flame is a laminar premixed front, the TF model propagates it at the laminar flame speed exactly like in a G equation approach[1]. However, this flame propagation is due to the combination of diffusive and reactive terms which can also act independently so that quenching (near walls for example) or ignition may be simulated. Fully compressible equations may also be used as required to study combustion instabilities.

Obviously, thickening the flame front also leads to a modified interaction between the turbulent flow and the flame: subgrid scale wrinkling must be reintroduced.
This effect can be studied and parametrized using an efficiency function \( E \) derived from DNS results [5, 18, 29]. This efficiency function measures the subgrid scale wrinkling as a function of the local subgrid turbulent velocity \( u'_{\Delta_e} \) and the filter width \( \Delta_e \). In practice, the diffusion coefficient \( D_k \) is replaced by \( E F D_k \) and the preexponential constant \( A \) by \( AE \) so that the conservation equation for species \( k \) is:

\[
\frac{\partial \rho Y_{th}^k}{\partial t} + \frac{\partial \rho u Y_{th}^k}{\partial x} = \frac{\partial}{\partial x} \left( \rho E F D_k \frac{\partial Y_{th}^k}{\partial x} \right) + \frac{E}{F} \omega_k \left( Y_{th}^j, T'^{th} \right)
\]  

This equation allows the turbulent flame to propagate at a turbulent speed \( s_T = Es_L^{0} \) while keeping a thickness of the order of \( \delta_L^{1} = F \delta_L^{0} \). In laminar regions, \( E \) goes to unity, and Eq. (4) simply propagates the front at the laminar flame speed \( s_L^{0} \).

A central ingredient of the TF model is the subgrid scale wrinkling function \( E \). For this work, the initial model of Colin et al. [5] was used to express \( E \) as a function of the local filter size \( \Delta_e \), the local subgrid scale turbulent velocity \( u'_{\Delta_e} \), the laminar flamespeed \( s_L^{0} \) and the laminar flame thicknesses \( \delta_L^{0} \) and \( \delta_L^{1} \):

\[
E = \frac{\Xi(\delta_L^{0})}{\Xi(\delta_L^{1})} = \frac{1 + \alpha \Gamma \left( \frac{\Delta_e}{\delta_L^{1}}, \frac{u_{\Delta_e}'}{s_L^{0}} \right) \frac{u_{\Delta_e}'}{s_L^{0}}}{1 + \alpha \Gamma \left( \frac{\Delta_e}{\delta_L^{0}}, \frac{u_{\Delta_e}'}{s_L^{0}} \right) \frac{u_{\Delta_e}'}{s_L^{0}}}
\]  

where the function \( \Gamma \) corresponds to the integration of the effective strain rate induced by all scales affected by the artificial thickening, i.e. between the Kolmogorov \( \eta_K \) and the filter \( \Delta_e \) scales. \( \alpha \) is a model parameter which scales as \( \alpha \propto Re^{-\frac{1}{2}} \) (Colin et al. [5]). \( \Gamma \) is written as:

\[
\Gamma \left( \frac{\Delta_e}{\delta_L^{1}}, \frac{u_{\Delta_e}'}{s_L^{0}} \right) = 0.75 \exp \left[ -\frac{1.2}{\left( \frac{u_{\Delta_e}'}{s_L^{0}} \right)^{0.3}} \right] \left( \frac{\Delta_e}{\delta_L^{1}} \right)^{2/3}
\]  

The subgrid scale turbulent velocity is evaluated as: \( u'_{\Delta_e} = 2\Delta_e^3 |\nabla^2 (\nabla \times \vec{u})| \), where \( \Delta_e \) is the grid size. This formulation provides an estimate of the subgrid scale velocity which is unaffected by dilatation [5]. Note that the filter size \( \Delta_e \) may differ from \( \Delta_e \). It was suggested by Colin [5] to choose \( \Delta_e = 10\Delta_e \).

The LES studies of Angelberger et al. [3] and Colin et al. [5] as well as various other tests have shown that Eq. (5) was adequate to predict subgrid scale wrinkling. In this work, a thickening factor \( F = 25 \) was used. Eq. (5) was developed and tested with single-step chemical schemes. Since the present study uses a two-step mechanism, additional DNS were performed to study the TF approach combined
with a two-step chemical scheme [30] and to check whether the existing efficiency functions proposed in [5, 18] or [29] could be used without modification. Results showed that the two chemical reaction rates follow exactly the same evolution during these flame vortex interactions. These DNS suggest that, for the investigated range of parameters, the premixed flame acts as a flamelet distorted by flow motions even for low values of the length scale ratio \( r/(F\delta L) \), where \( r \) is the length scale on the vortices interacting with the flame front. Moreover, the effective strain rates induced by the vortices on the flame front and extracted from these DNS are in close agreement with [5, 18] findings. Accordingly, the efficiency functions derived in [5, 18, 29] were used without any modifications with the present two-step chemical scheme.

4 TWO-STEP CHEMISTRY

The complexity of the chemical scheme used in a TF model must remain limited because all species are explicitly resolved. Up to now, only simple one-step chemical schemes have been used in TF models [3, 5]. In the present study, a two-step scheme is introduced to capture \( CO \) and predict more adequate flame temperatures as an intermediate step towards more complex schemes (typically four-step schemes such as [31]).

The chemical scheme (called 2sCM2) takes into account six species (\( CH_4, O_2, CO_2, CO, H_2O \) and \( N_2 \)) and two reactions:

\[
CH_4 + \frac{3}{2} O_2 \rightarrow CO + 2H_2O \tag{7}
\]

\[
CO + \frac{1}{2} O_2 \leftrightarrow CO_2 \tag{8}
\]

The first reaction (7) is irreversible whereas the second one (8) is reversible and leads to an equilibrium between \( CO \) and \( CO_2 \) in the burnt gases. The rates of reaction (7) and (8) are respectively given by:

\[
q_1 = A_1 \left( \frac{\rho Y_{CH_4}}{W_{CH_4}} \right)^{n_{CH_4}} \left( \frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{O_2}} \exp \left( -\frac{E_{a1}}{RT} \right) \tag{9}
\]

\[
q_2 = A_2 \left[ \left( \frac{\rho Y_{CO}}{W_{CO}} \right)^{n_{CO}} \left( \frac{\rho Y_{O_2}}{W_{O_2}} \right)^{n_{O_2}} - \left( \frac{\rho Y_{CO_2}}{W_{CO_2}} \right)^{n_{CO_2}} \right] \exp \left( -\frac{E_{a2}}{RT} \right) \tag{10}
\]

where the parameters are provided in Table 1.

Transport by molecular diffusion also requires attention: laminar flame codes such
as PREMIX use polynomial fits for diffusion coefficients $D_k$. This technique is precise but expensive and may be replaced by a simpler approximation based on the observation that the individual Schmidt numbers of species $S^k_c = \nu/D_k$ are almost constant in many air / hydrocarbon flames. Therefore, in AVBP, the diffusion coefficient $D_k$ of species $k$ is obtained as $D_k = \nu/S^k_c$ where $\nu$ is the viscosity and $S^k_c$ the fixed Schmidt number of species $k$. The Schmidt number values used in the present simulations are given in Table 2. In most cases, these values correspond to the PREMIX values measured in the burnt gases. The Prandtl number is set to 0.68. With this parameter set, the agreement between flame profiles obtained using AVBP or PREMIX with the same chemical scheme is excellent (Fig. 1).

This scheme is directly implemented into the LES code. Its first advantage compared to a single-step scheme is to provide more accurate adiabatic flame temperatures. Fig. 2 compares the maximum flame temperatures obtained with AVBP and PREMIX using the full GRI mechanism. For 2sCM2, AVBP and PREMIX predict the same maximum flame temperature, confirming that the thermodynamical data of AVBP is correct. 2sCM2 overestimates the maximum flame temperatures compared to GRImech by 100 K for rich cases but is very accurate for lean mixtures. The laminar flame speeds are also well predicted on the lean side (Fig. 3) but deviate from the exact results for rich cases. For the turbulent case presented below, an equivalence ratio of 0.5 was used so that the 2sCM2 predictions are very precise.

5 Configuration

An important objective of this study was to investigate the limits of present computer capabilities to perform LES of combustion in realistic geometries. An industrial gas turbine burner is considered here. The CAD data was provided by Siemens PG. The grid contains 2381238 cells. Fig. 4 shows the main features of the burner: a central axial swirler (colored in dark) is used to inject and swirl air and, for certain regimes (not studied here), non premixed fuel. In addition, six small tubes (not visible on this figure) can be used to generate pilot flames but they were not fed during the present computation. The main part of the combustion air as well as fuel (through holes located on both sides of the vanes used for swirling) is injected by the diagonal swirler. Its external surface is visualized in Fig. 4 by a wire type surface. For the present study, both axial and diagonal swirlers are fed with premixed air.

6 Experimental Techniques

A single SIEMENS burner (scale 1:1) is mounted on an atmospheric test rig. The combustion chamber has a square cross section with a truncated pyramid shape at
the exit. Both the casing and the chamber walls allow optical access for velocity measurements by LDA. The burner is fired with natural gas (assumed to be mostly methane), and the air is pre-heated to 673K. The thermal power varies between 420kW (at $\Phi = 0.5$) and 810kW (at $\Phi = 0.83$).

Measurements were performed at ITS Karlsruhe to characterize:

- the cold fbw velocity field in terms of mean and RMS velocities using LDA techniques,
- the hot fbw velocity field in terms of mean and RMS components as well as the mean temperature field using thermocouple data\(^1\).

Measurements are performed in transverse cuts and at the outlet of the diagonal swirler as represented in Fig. 6. For the cold fbw, data are gathered over 15 cuts ranging from $x/R = 0.37$ to $x/R = 4.17$, where $R$ is the radius of the burner outlet. For the case with combustion, there are 6 cuts ranging from $x/R = 0.7$ to $x/R = 4.32$.

An important difference must be pointed out regarding the comparison between LES and experimental data: the LES is performed assuming perfectly premixed reactants (at the same equivalence ratio $\phi = 0.5$) in both diagonal and axial swirlers. In the real experiment, methane is injected through the vanes of the diagonal swirler and upstream of the vanes of the axial swirler. Tests conducted at ITS Karlsruhe have shown that, for the regime studied here, the injection of methane through the diagonal swirler does not change the fbw topology and affects the mean and RMS data in a very limited manner. Obviously, in certain regimes, the methane injected through the axial swirler acts as a pilot flame which is essential for flame stability: this is not the case for the regime considered here and the comparison is performed as if all reactants would also be premixed in the experiment.

### 7 INLET CONDITIONS

A major issue in LES calculations is to specify boundary conditions. Since the axial burner is fully computed, the fbw in Section A (Fig. 6) is introduced along the $x$ axis only without swirl and the computation should produce the right fbw field at the burner mouth. The main problem is then to specify inlet conditions for the diagonal swirler (Section D in Fig. 6). Section D is located downstream of the vanes of the diagonal swirler and velocities could not be measured at this location. The LES however starts in section D and the inlet velocity profiles in this section are adjusted to match the first measurement section (Cut 1d in Fig. 6) in the burner

\(^1\) The time response of the thermocouple was not sufficient to provide RMS temperature data.
under non-reacting cases.

Velocity measurements have been performed in various sections displayed on Fig. 6. The swirling velocity $W$ and the velocity $U_{22}$ normal to a plane parallel to the diagonal swirler exit plane (at an angle of 22 degrees compared to the vertical axis) are measured in the test section located close to the burner nozzle (cut 1d). Distances and velocities are respectively scaled by the burner radius $R$ and the bulk velocity $U_{\text{bulk}}$ defined by $U_{\text{bulk}} = \dot{V} / \pi R^2$ where $\dot{V}$ is the total volume flow rate through the burner.

Average profiles of axial and radial velocities at the exit of the diagonal burner are displayed in Fig. 7 and 8 (cut 1d in Fig. 6). In figures, symbols (○) denote experimental data while LES results are plotted with solid lines (–). No fluctuating velocity components are added to the inlet conditions: this incoming turbulence can be neglected compared to the turbulent activity in the chamber which is due to the very high velocity gradients created by the swirling motion in the dump plane of the chamber. This is confirmed in the next section by the comparison of experimental and computational fluctuating velocity components in the chamber.

8 NON REACTING FLOW RESULTS

8.1 Averaged fields

Once the inlet conditions have been set, LDV measurements (○) are compared to averaged LES results (——) at different downstream locations $x$ in the combustor (Fig. 9 to 12). In Fig. 9 (axial velocity profiles) and 10 (swirling velocities), LES data are averaged over about 36 ms corresponding to two flow times through the entire combustion chamber at the bulk velocity. Only 6 downstream locations are displayed for clarity but 15 were investigated.

The overall agreement between LES and experimental data is excellent. The size, shape and intensity of the recirculation zone are well predicted, as well as the overall spreading of the turbulent swirling jet. All results are displayed for the whole size of the combustion chamber and not only for one half chamber to evidence symmetry defaults. Since the chamber is square and the injection device axisymmetric, average velocities are expected to be symmetrical versus the $x$-axis. However both experimental data and LES results are not perfectly symmetrical, especially downstream. This finding (which is quite usual in these fbws) may indicate a lack of sampling of LES data but may also be due to an intrinsic difficulty in such fbws to follow the symmetry of the geometry.

Concerning the RMS profiles (Fig. 11 and 12), only the resolved part of the fluctu-
ations is taken into account here. This demonstrates that for this fbw, most of the unsteady motion lies in large structures which are very well predicted by LES methods. Cut $x/R = 0.37$ in Fig. 12 shows that the largest fluctuations of the swirling component are located on the axis, and reach up to 60% of the bulk velocity. This will be explained in the following section “Unsteady flow analysis” by the presence of a coherent structure.

An additional quantity which can be extracted directly from this compressible LES is the RMS pressure $P'$, both in the chamber and on its walls. Fig. 13 shows that the largest pressure oscillations are found in front of the axial swirler outlet. Fairly high pressure levels ($2500 \text{Pa}$) are observed inside the combustor at the swirler outlet but they do not propagate to the walls. Most of these pressure oscillations are due to the precessing vortex described in the next section.

8.2 Unsteady flow analysis

Swirling fbws can exhibit a very large range of topologies, mainly depending on the swirl number (see the review on vortex breakdown in [32]). For high values of the swirl number, the central recirculation zone may oscillate at a given frequency. This phenomenon is often referred to as precessing vortex core (PVC). Fig. 14 shows the topology of a precessing vortex core. The vortex aligned with the axis of the chamber (due to the swirl) breaks down at the stagnation point $S$ in a spiral form. In the present regime, the fbw inside the spiral is recirculated. The entire structure rotates around the axis of the chamber, causing large perturbations. The present LES captures this phenomenon: on the burner axis, at point $A1$ (Fig. 6), the velocity component $W$ oscillates with time (Fig. 15) at a frequency $f_{LES} = 280 \text{ Hz}$. Indeed, if the fbw were axisymmetric, $W$ would be zero on the axis of the burner. The computed Strouhal number $St = (2R/f_{LES})/U_{bulk} = 0.63$ is typical of swirling fbws [33]. The value of $f_{LES}$ is also very close to that obtained experimentally at ITS: $f_{exp} = 260 \text{ Hz}$.

Note that the LES gives an additional information on the temporal evolution of the spiral: the sense of winding of the spiral and the sense of rotation of the whole spiral, as a structure, is that of the surrounding swirling fbw. Fig. 17 is an instantaneous visualisation of the PVC in the cold fbw.

9 REACTING FLOW RESULTS

Reacting cases are computed starting from a cold fbw solution. Fresh premixed gases (equivalence ratio $\phi = 0.5$) are injected through the diagonal and the axial swirler. Both fbws, coming from the compressor in the actual gas turbine, enter
the combustion chamber of the ITS burner after being preheated electrically to a temperature $T = 673K$. As the actual ignition process is not described here, the chemical reaction is numerically started by filling the combustion chamber with hot fully burned gases. Note however that the pressure increases by 25 % and the exit velocity Mach number goes up to 0.4 in the outlet contraction during the transient ignition phase [30].

9.1 Unsteady flow analysis

A three-dimensional visualization of the reacting flow field is displayed in Fig. 18: the temperature isosurface at $T = 1000K$ shows the topology of the flame surface and illustrates the turbulent nature of the flame / flow interaction. Pockets of fresh gases are periodically shed from the main flame zone and burn downstream. A central core of hot gases is stabilized along the burner axis by the recirculation zone induced by swirl: this core is attached to the face of the axial swirler (Fig. 19). The field of axial velocity, normalized by $U_{bulk}$, is displayed in Fig. 20 with isocontours of heat release.

A specific feature of the reacting case is that the PVC structure evidenced in the cold flow cases disappears when combustion is turned on. Fig. 21 is a record of the velocity in the horizontal central plane ($W$) at point A1 (Fig. 6) after ignition. The velocity signal oscillates around zero as the core of the recirculation zone moves around the axis of the combustion chamber. After a few periods, the PVC motion vanishes. This observation obtained from LES data is confirmed by experimental results.

9.2 Averaged fields

In this section, the mean results of the LES (——) are compared to experimental data (○). Fig. 22 to 26 show the measurements conducted only in one half of the combustion chamber.

Mean temperature profiles obtained from LES are compared to experimental data in Fig. 22. The thickness of the turbulent flame brush is slightly underestimated (see $x/R = 0.7$ in Fig. 22). However, the agreement between LES and experimental data is good, and quantities which are important for the turbine design, are well reproduced:

- the length of the flame is very well predicted,
- the burnt gas temperature is very slightly overpredicted by the LES, mainly due to the non-adiabaticity of the experiment, while the LES assumes adiabatic walls.
Mean axial and tangential velocity profiles are respectively given in Fig. 23 and 24. The overall agreement is fairly good but the underestimation of the lateral expansion of the jet must be pointed out. RMS profiles of both axial and tangential velocities are plotted in Fig. 25 and 26. The level of the fluctuations is well predicted. Though the shape and level of axial velocity RMS fluctuations have not changed significantly between cold and hot flow (Fig. 11 and 25), swirling velocity RMS fluctuations are very different on the first profiles (Fig. 12 and 26). At $x/R = 0.37$ for example, the RMS swirling speed is $U'/U_{bulk} \approx 0.7$ on the burner axis ($y = 0$) on Fig. 11 for the cold flow, and it decreases to $U'/U_{bulk} \approx 0.1$ on Fig. 26 with combustion. This confirms that the fluctuations of azimuthal component are strongly reduced with combustion due to the suppression of the PVC structure, and the LES captures this effect with accuracy.

Fig. 27 is the iso-surface $T = 1000K$ of the mean solution. The wakes of the six blades of the axial swirler are clearly visible, showing the influence of the vanes of the axial swirler.

The analysis of the pressure fluctuations $P'$ in a longitudinal cut reveals another important difference between cold and reacting flow: the pressure fluctuations observed in the cold flow (see Fig. 13) in front of the axial swirler disappear when combustion is turned on (Fig. 28). This is consistent with the suppression of the PVC when combustion is started: the cold flow unsteady pressure field is dominated by the presence of the PVC while the reacting flow inhibits the PVC. Plotting $P'$ on the walls of the combustion chamber (Fig. 29) shows that an acoustic mode of the chamber is now excited. The shape of this mode seems to be that of a quarter-wave length in $x$ direction, and half-wave length in both cross directions. Fig. 30 displays the pressure signals versus time for four points $C_1$, $C_2$, $C_3$ and $C_4$ located in the corner recirculation zones (see Fig. 5). The phase difference between consecutive pressure tracers is $\pi/2$: this indicates that the acoustic mode is rotating around the main burner axis. The frequency of this mode is 1200 Hz. Its coupling with combustion has not been analysed yet.

10 CONCLUSIONS

A computation of a full burner of a premixed gas turbine installed in a laboratory rig was performed using LES for both non-reacting and reacting cases. The flame is described using a two-step chemical scheme for methane / air combustion combined with the thickened flame (TF) model. LES results are validated from velocity and temperature measurements performed at University of Karlsruhe. The overall agreement with experiment is very good both for cold flow and for reacting conditions. A strong precessing vortex core (PVC) is observed for the non-reacting flow. This vortex disappears when combustion is activated. Unsteady pressure fields are also very different for cold and reacting flow: maximum pressure oscillations are
observed in the PVC zone for the cold flow; with combustion, the pressure oscillations maxima are located at the chamber walls and have an acoustic structure corresponding to a coupled transverse-longitudinal mode. More generally, this study demonstrated that LES for reaction flows in complex geometries has now reached sufficient maturity to bring original information on such complex combustion devices.

11 ACKNOWLEDGEMENTS

Certain numerical simulations have been conducted on the computers of CINES and IDRIS french national computing centers.

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12 REFERENCES


Table 1
Rate constants for the 2sCM2 scheme: the activation energies are in cal/moles and the preexponential constants in cgs units.

<table>
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<tr>
<th>$A_1$</th>
<th>$n_{CH_4}$</th>
<th>$n_{O_2}$</th>
<th>$E_{a1}$</th>
<th>$A_2$</th>
<th>$n_{CO}$</th>
<th>$n_{O_2}$</th>
<th>$n_{CO_2}$</th>
<th>$E_{a2}$</th>
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<td>34500</td>
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<td>1</td>
<td>0.5</td>
<td>1</td>
<td>12000</td>
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Table 2
Schmidt numbers.

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<th>$CH_4$</th>
<th>$CO_2$</th>
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<th>$O_2$</th>
<th>$H_2O$</th>
<th>$N_2$</th>
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<tbody>
<tr>
<td>0.68</td>
<td>0.98</td>
<td>0.76</td>
<td>0.76</td>
<td>0.6</td>
<td>0.75</td>
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Fig. 1. Comparison of AVBP and PREMIX for a laminar one-dimensional flame at $\phi = 0.5$. The fresh gas temperature is 673 K.

Fig. 2. Burnt gas temperature (K).

Fig. 3. Laminar Flame speed $s_L^0$ ($m.s^{-1}$).
Fig. 4. Burner: the vanes of the diagonal swirler are not computed.

Fig. 5. Burner mounted on ITS combustion chamber.

Fig. 6. Burner mounted on ITS combustion chamber: location of LDV measurements.

Fig. 7. Normalized velocity $U_{22}/U_{bulk}$ at the exit of the diagonal swirler (Cut 1d).

Fig. 8. Normalized swirl velocity $W/U_{bulk}$ at the exit of the diagonal swirler (Cut 1d).
Fig. 9. Cold flow mean axial velocity ($U/U_{bulk}$).

Fig. 10. Cold flow mean swirling velocity ($W/U_{bulk}$).
Fig. 11. Cold flow axial velocity fluctuations ($U'/U_{bulk}$).

Fig. 12. Cold flow swirling velocity fluctuations ($W'/U_{bulk}$).
Fig. 13. RMS pressure fluctuations $P'$ in a longitudinal cut for the cold flow (Pa).

Fig. 14. Topology of a precessing vortex core (PVC).
Fig. 15. Cold flow: $W$ velocity at point A1.

Fig. 16. Cold flow: Fourier transform of $W$ velocity signal at point A1.

Fig. 17. Visualisation of the PVC structure by a Pressure iso-surface.
Fig. 18. Axial swirler vanes and isosurface of temperature ($T = 1000K$) colored by velocity modulus (see full animation at http://www.cerfacs.fr/cfd/FIGURES/MOVIES/flame-ITS.mov).
Fig. 19. Instantaneous temperature field and contours of zero axial velocity in a longitudinal cut of the burner.

Fig. 20. Instantaneous axial velocity field and contours of reaction rate in a longitudinal cut of the burner.
Fig. 21. Reacting flow: $W$ velocity signal at point A1 (Fig. 6) after ignition.

Fig. 22. Reacting flow mean temperature (K).
Fig. 23. Reacting flow mean axial velocity ($U/U_{bulk}$).

Fig. 24. Reacting flow mean swirling velocity ($W/U_{bulk}$).
Fig. 25. Reacting flow, axial velocity fluctuations ($U'/U_{bulk}$).

Fig. 26. Reacting flow, swirling velocity fluctuations ($W'/U_{bulk}$).
Fig. 27. Mean flow. Axial swirler vanes and isosurface of temperature ($T = 1000K$) colored by velocity modulus.
Fig. 28. RMS pressure fluctuations $P''$ in a longitudinal cut for the hot flow (Pa).

Fig. 29. RMS pressure fluctuations $P''$ on the walls of the chamber for hot flow (Pa).
Fig. 30. Pressure signal versus time in the corner recirculation zones of the chamber. A rotating acoustic mode is evidenced (see full animation at http://www.cerfacs.fr/cfd/FIGURES/MOVIES/P_traces_trans-ITS.mov).