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Chemical kinetics modeling and LES combustion model effects on a perfectly premixed burner

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Abstract

Chemical kinetics modeling and coupling with turbulent combustion models for compressible Large Eddy Simulations (LES) is a critical issue. Accurate flow predictions can only be guaranteed if the coupling is well mastered. In a first attempt to qualify the effect of each model, the case of a lean premixed swirled combustor with comprehensive measures is targeted (species mass fractions and temperature fields). For the investigation, two turbulent combustion models are considered. The first model relies on a presumed PDF approach coupled to a look-up chemistry table obtained with a reduced chemical scheme. The second model makes use of the thickened flame approach using the same reduced chemical scheme but with reaction rates computed explicitly as the computation advances. Then, to estimate kinetic schemes reduction effects, the first model is compared to a third one, with the same PDF approach, but coupled to a look-up chemistry table obtained with a complete chemical scheme. All LES are very close to each other. The main difference between the different predictions relies on CO mass fractions. Although they are all able to return good outlet mass fractions, CO values inside the flame are different depending on the model used. ***To cite this article: G. Albouze et al., C. R. Mecanique 337 (2009).***

Résumé

Effets de la modélisation de la cinétique chimique et des modèles de combustion LES sur un brûleur parfaitement prémélangé. La modélisation de la cinétique chimique et le couplage avec les modèles de combustion turbulente pour la simulation aux grandes échelles doivent être maîtrisés pour garantir les prédictions d'écoulements de chambres de combustion. Deux modèles de combustion turbulente sont utilisés. Le premier repose sur une approche de PDF présumée couplée à une table chimique obtenue avec une schéma cinétique réduit. Le second modèle utilise l'approche de flamme épaissie et le même schéma cinétique réduit, mais dont les taux de réactions sont calculés explicitement. Puis, pour estimer les effets de réduction de cinétique chimique, le premier modèle est comparé à un troisième, avec la même approche PDF, mais couplée à une table obtenue avec un schéma cinétique complet. Des mesures expérimentales complètes (température et de fractions massiques des espèces) réalisées sur un brûleur prémélangé pauvre sont comparées aux résultats de simulation. Tous les résultats LES sont proches les uns des autres, la différence principale se trouvant sur les fractions massiques de CO. ***Pour citer cet article : G. Albouze et al., C. R. Mecanique 337 (2009).***

Keywords: Combustion; Chemical kinetics; LES combustion model

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Mots-clés : Combustion ; Cinétique chimique ; Modèle de combustion LES

1. Introduction

With the permanent increase of computer resources, Large Eddy Simulations (LES, [1–7]) are commonly used on turbulent complex, reacting or not, Computational Fluid Dynamics (CFD) applications. LES are the best compromise between feasibility and physical accuracy. Recent applications prove that they are able to capture many physical phenomenons, including instabilities or acoustic activity [8–12]. However, reactive LES can be performed by coupling different chemical kinetics methods, such as reduced kinetics or complex tabulated chemistry with different LES turbulent combustion models and the optimal approach is still not clear especially if pollutant emissions are to be accurately predicted.

In a first attempt to qualify and understand the effect of each model, the case of a lean premixed swirled combustor with comprehensive measures is targeted (species mass fractions and temperature LES fields, averaged and RMS, are compared with experimental data). For the investigation, two turbulent combustion models are gauged. The first model relies on a presumed PDF approach coupled to a look-up chemistry table obtained a priori with a reduced chemical scheme [13–17]. The second model makes use of the thickened flame approach (TFLES) using the same reduced chemical scheme but with reaction rates that are computed explicitly as the computation advances [1,18,19]. Then, to estimate kinetic scheme reduction effects, the first model is compared to a third one, with the same PDF approach, but coupled to a look-up chemistry table obtained a priori with a complete chemical scheme.

The next part explains the common parameters of every performed LES, i.e. the LES solver, the combustor geometry, the computational domain, the mesh and boundary conditions. Then, turbulent combustion models and chemical kinetic modelings are described and compared on a perfectly premixed monodimensional flame. LES results are shown in the following part and turbulent combustion models are specifically compared, before assessing the impact of the chemical kinetics.

2. Large eddy simulations of the swirled premixed burner

2.1. Common parameters

The massively-parallel LES solver used in this study has been successfully used for several CFD applications [3,8–11,19–25]. It solves the full compressible Navier–Stokes equations on hybrid (structured and unstructured) grids with third-order spatial and temporal accuracy [23,26] and uses real thermo-chemistry for turbulent combustion applications.

The combustor investigated here has been described and studied, experimentally [27–29] and numerically [8,16, 30]. It is derived from an industrial design by Turbomeca (Fig. 1) and LES have, in particular, proven their capabilities on this complex combustor, with the same computational domain, mesh and type of boundary conditions, with TFLES/reduced chemistry [8] and with PCM-FPI [16].

The combustor can be divided into 4 distinct parts. The first part is the plenum, where an air flow is injected through one large hole. The second part is the injector, where the air flow is swirled by 12 radial vanes, inside which methane is injected through 1 mm holes (one methane jet per vane). The third part is the combustion chamber, which has a square cross section (86×86 mm^2) and quartz wall to permit the measurements to be performed. The fourth part is the exhaust pipe, with a 40 mm diameter and which leads to the atmosphere.

Several regimes have been studied experimentally [27]. The "2a" has been chosen in this study. It corresponds to an equivalence ratio of 0.83, an air flow rate of 12.237 g/s, a methane flow rate of 0.5983 g/s, and a thermal power of 30 kW. It is a stable regime, where Raman measurements have been performed. Thus, full average and RMS experiments data can be compared to LES.

Domain, mesh and boundary conditions at walls and at the outlet are strictly the same as in [8]. The domain begins with the plenum and ends with an atmosphere to ensure that the boundary conditions are well controlled. In the experiment, air and methane are injected separately. Air enters the plenum and methane is injected directly inside the injector vanes. For LES, it is supposed that mixing is fast enough for methane and air to be perfectly premixed when arriving to the flame. Thus, methane injection has been suppressed and an equivalent methane/air mixture is

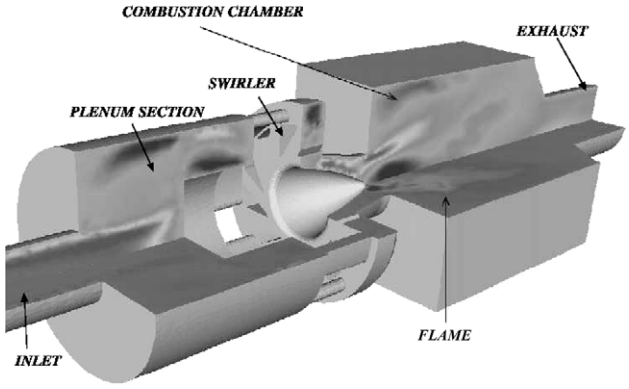

Fig. 1. Global view of the burner and combustion chamber.

injected at the plenum inlet. A recent study [27] has shown strong mixture fraction heterogeneities inside the combustion chamber. The perfectly premixed hypothesis that has been done here appears to be in disagreement with these observations. Other LES are actually performed on the same test case, without the perfectly premixed assumption. The mesh is unstructured and contains about 3 millions elements. No-slip adiabatic conditions are imposed at all walls of the chamber. The inlet is a fixed velocity section and the outlet is a constant pressure surface [1]. At the inlet of the plenum, only gas composition and mass flux have been changed, to a perfectly premixed equivalence ratio equal to 0.83 and mass flux equal to 0.012835 kg/s. More details can be found in [8].

2.2. Turbulent combustion models

Two different turbulent combustion models are compared. The first one is the Thickened Flame (TFLES) model, used with a dynamic efficiency function [18,19]. Flames are artificially thickened, so as to resolve the flame fronts on a LES mesh, by multiplying diffusion and dividing reaction rates by a thickening factor F. Thus, flames are thickened by a factor F, but flame velocities are conserved [1]. An efficiency function is added to the TFLES model, so as to correct the reduction of flame surface induced by the TFLES model. The second turbulent combustion LES model is the Presumed Conditional Moments (PCM) model [13–15]. With this approach and contrarily to the TFLES model, the filtered reaction rates are calculated as the integration of a laminar reaction rates multiplied by a joint PDF [1]. Details about PCM can be found in [16,17].

2.3. Chemical kinetics modeling

Two types of chemistry modelings are compared: reduced kinetic schemes and tabulated chemistry. The reduced kinetic scheme is the two step scheme used in [8]. It takes into account six species (CH_4, O_2, CO_2, CO, H_2O and N_2) and two reactions [3]:

$$CH_4 + \frac{3}{2}O_2 \longrightarrow CO + 2H_2O \tag{1}$$

$$CO + \frac{1}{2}O_2 \longleftrightarrow CO_2 \tag{2}$$

The first reaction (1) is irreversible whereas the second one (2) is reversible and leads to an equilibrium between CO and CO_2 in the burnt gases and a correct prediction of product temperatures as well as laminar flame speed [3].

Complex tabulated chemistry corresponds to the FPI method described in [13,14,16,17,31–33]. Many kind of flames can be tabulated, depending on what is simulated. As the presented test case is perfectly premixed, tabulation is obtained from a perfectly premixed monodimensional flame, whose equivalence ratio is equal to 0.83. Two tables are generated, the first one with the complex kinetic scheme GRI-MECH (FPI case) and the second one with the two-

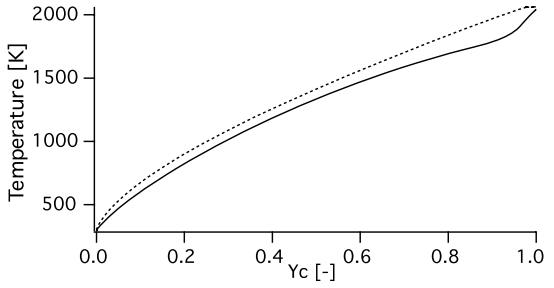

Fig. 2. Temperature as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

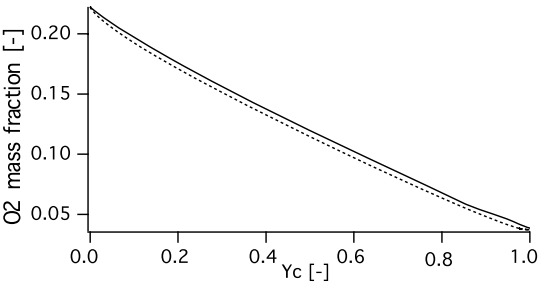

Fig. 3. O_2 mass fraction as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

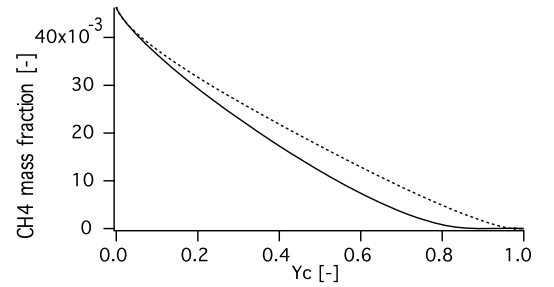

Fig. 4. CH_4 mass fraction as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

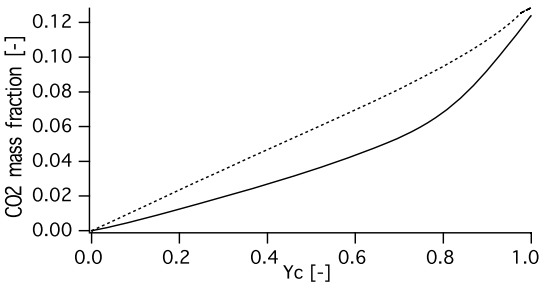

Fig. 5. CO_2 mass fraction as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

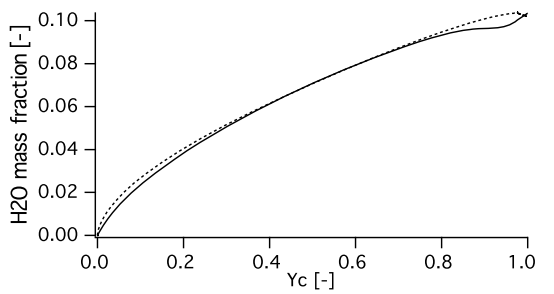

Fig. 6. H_2O mass fraction as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

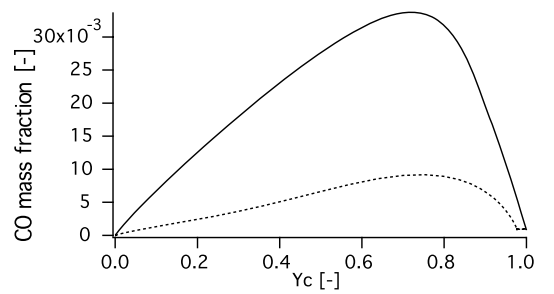

Fig. 7. CO mass fraction as a function of normalized progress variable for a premixed 1D flame. $\Phi = 0.83$. (—) GRI-MECH; (- - -) 2 steps scheme.

step reduced kinetic scheme used in [8] (two-step case). FPI tables are tabulations of major species mass fractions as a function of c, a normalized progress variable, defined by Eq. (3):

$$c = \frac{Y_{CO} + Y_{CO_2}}{(Y_{CO} + Y_{CO_2})_{\text{burnt gases}}} \tag{3}$$

$c = 0$ corresponds to fresh gases and $c = 1$ corresponds to burnt gases.

In the detailed FPI case, tabulated species are N_2, O_2, CH_4, CO_2, CO, H_2O, OH, H_2, H and C_2H_2. In the case where the table is obtained from the two-step reduced kinetic scheme, tabulated species are N_2, O_2, CH_4, CO_2, CO and H_2O. Both FPI tables are convoluted with the PCM model, so that they are finally tabulated as a function of c and c'^2.

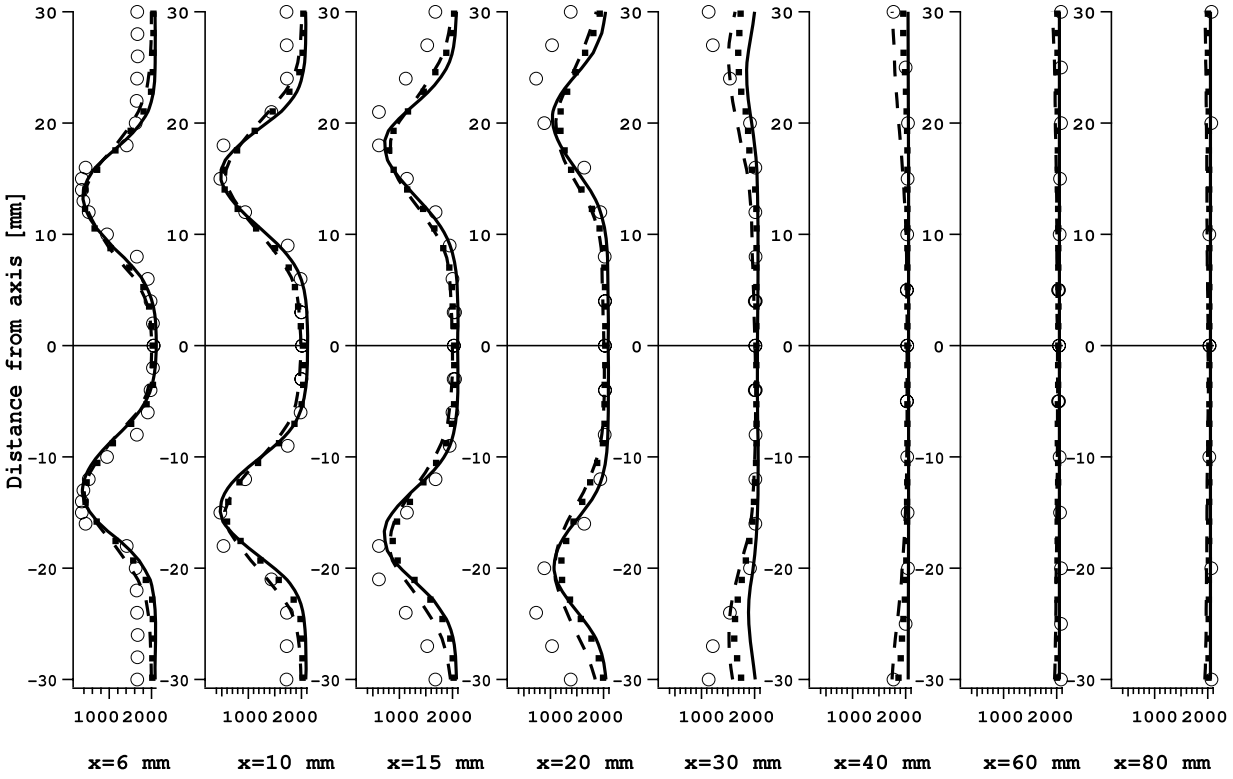

Fig. 8. Average temperature profiles. (○) Raman; (—) TFLES-2 steps; (– – –) PCM-2 steps; (■) PCM-FPI.

To better illustrate the implications of chemical kinetics, the two-step reduced kinetic scheme and complex chemistry are compared for a methane perfectly premixed 1D flame. The inlet temperature is set to 300 K and the equivalence ratio to 0.83, similarly to the value in the turbulent test case. The complex chemistry 1D flame is computed with Cantera [34].

Flame profiles can be observed on Figs. 2, 3, 4, 5, 6 and 7 where temperature and mass fractions are plotted as a function of c, the normalized progress variable.

For the two-step kinetic scheme, adiabatic temperature is 2059 K, while temperature given by complex chemistry is 2042 K (relative error less than 1%). For all mass fractions, boundary values are well respected but the flame structure differs slightly from the complex chemistry one. The biggest difference is found for the CO mass fractions. The second reaction of the mechanism (equilibrium between CO and CO_2) is able to produce good values of temperature, CO and CO_2 mass fractions in burnt gases, but CO values inside the flame are completely under-estimated. Maximum CO mass fraction in this premixed 1D flame is 9.18×10^{-3} for the two-step kinetic scheme and 33.7×10^{-3} for complex chemistry. Finally, the laminar flame speeds are evaluated at 0.300314 m/s with complex chemistry and 0.295638 with the two-step kinetic scheme (relative error around 1.56%).

3. Results

By combining turbulent combustion models and chemistry, three different simulations can be performed: PCM-FPI, PCM-reduced kinetic scheme and TFLES-reduced kinetic scheme.

The influence of the turbulent combustion model can be observed by comparing PCM-2 step and TFLES-2 step simulations (Section 3.1), whereas the influence of chemistry modeling can be observed by comparing PCM-FPI and PCM-2 step simulations (Section 3.2). Results are presented in Figs. 8 (mean temperature), 9 (mean CO mass fraction), 10 (RMS temperature), 11 (RMS CO mass fraction).

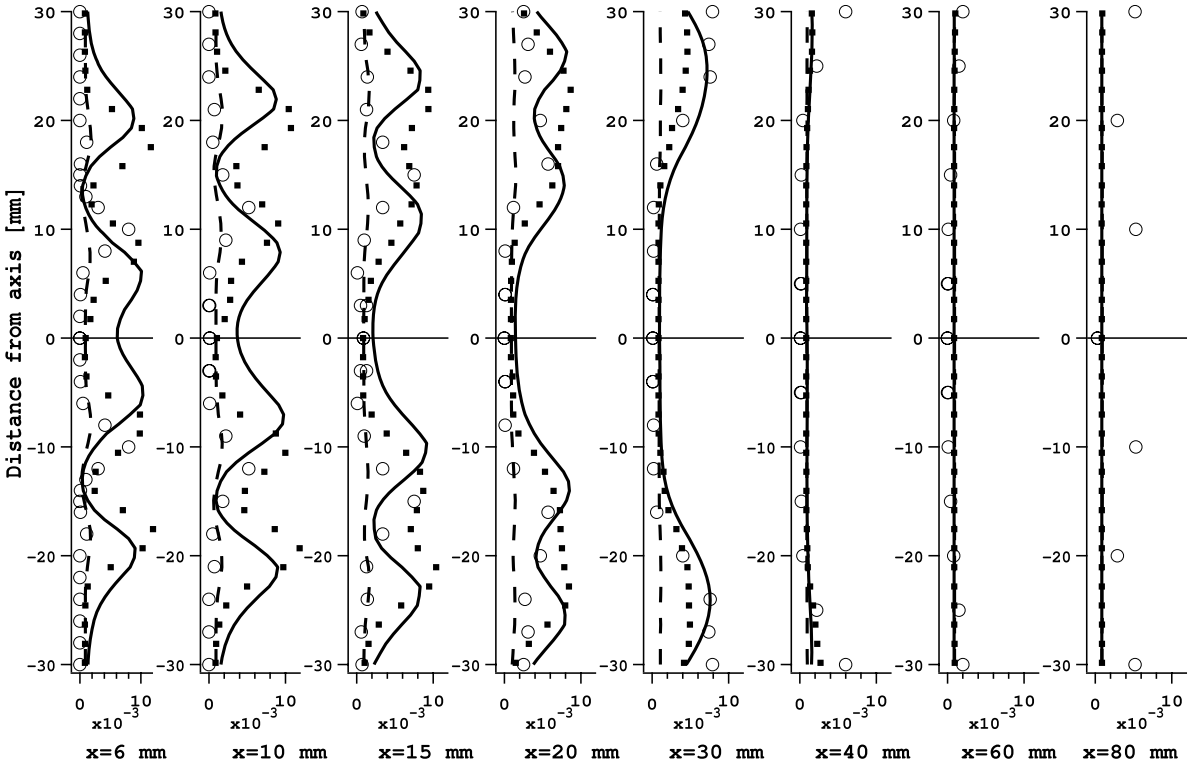

Fig. 9. Average CO mass fraction profiles. (○) Raman; (—) TFLES-2 steps; (– – –) PCM-2 steps; (■) PCM-FPI.

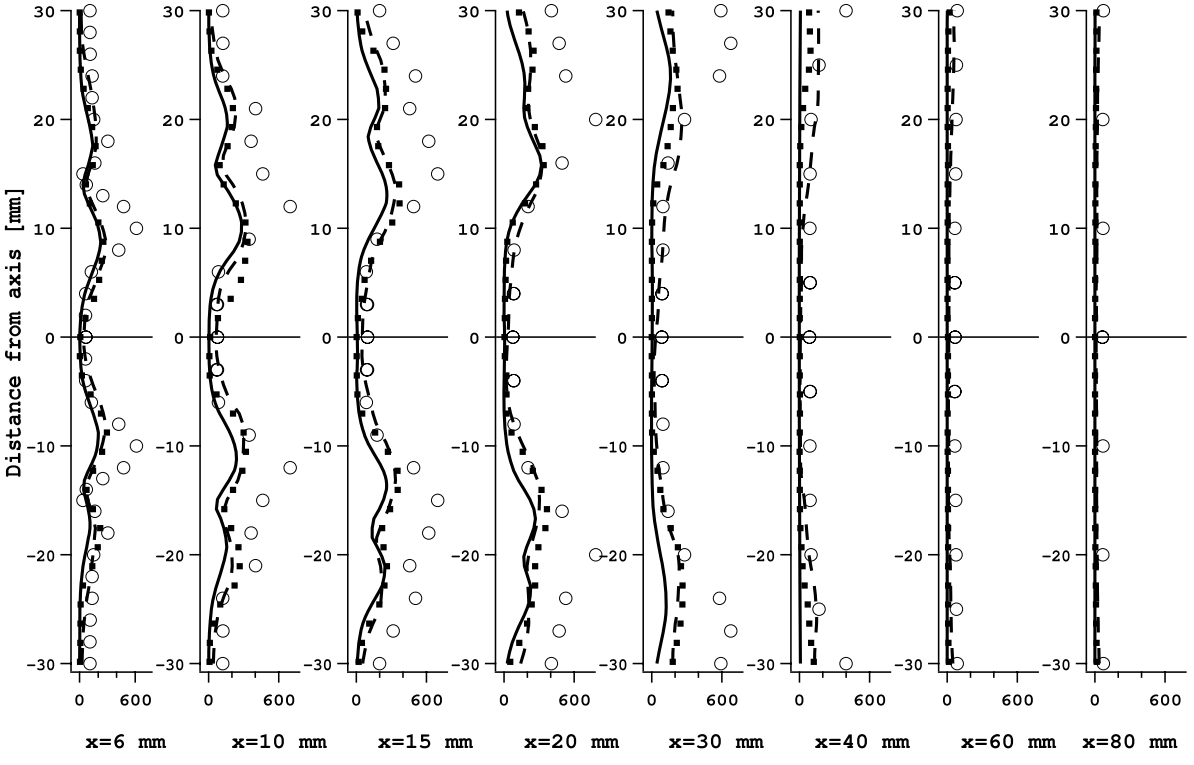

Fig. 10. RMS temperature profiles. (○) Raman; (—) TFLES-2 steps; (– – –) PCM-2 steps; (■) PCM-FPI.

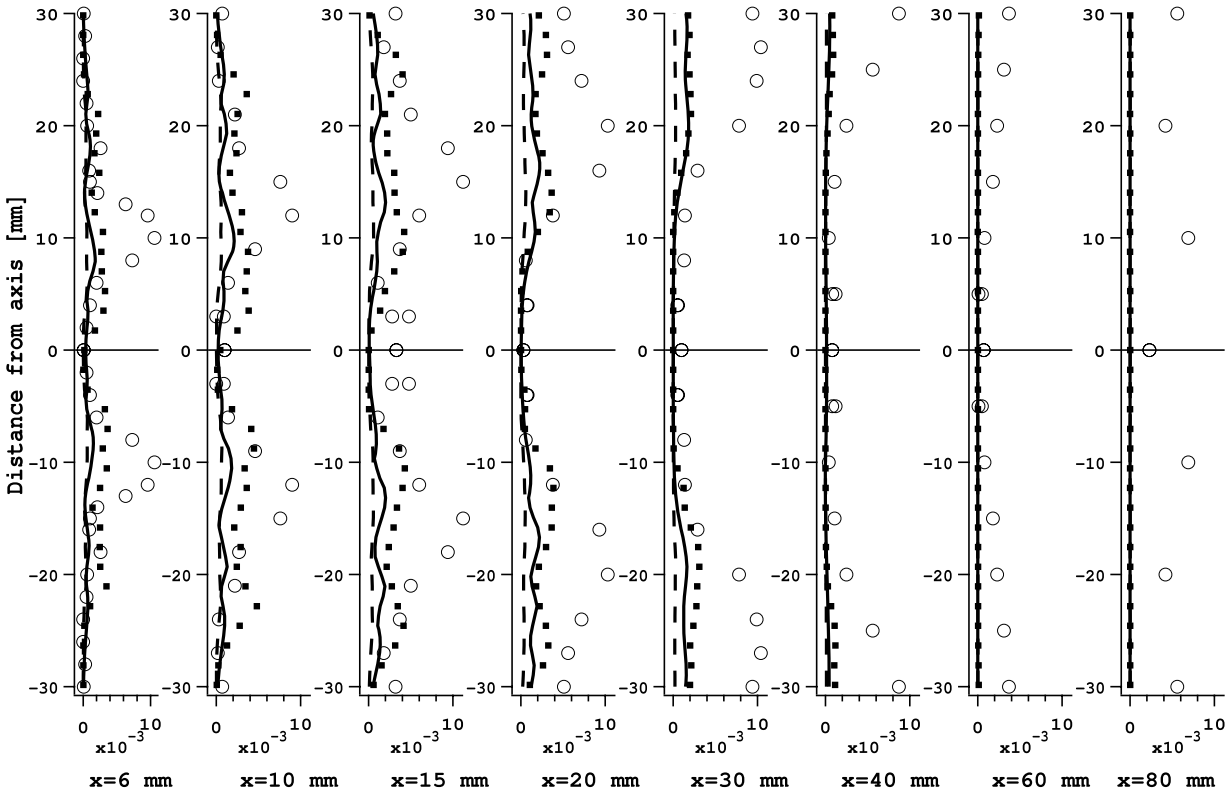

Fig. 11. RMS CO mass fraction profiles. (○) Raman; (—) TFLES-2 steps; (– – –) PCM-2 steps; (■) PCM-FPI.

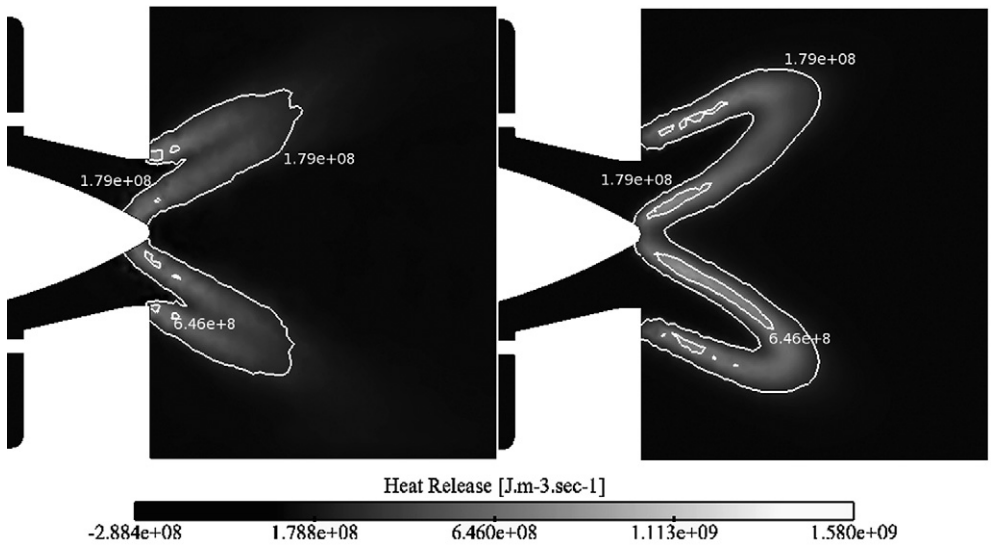

Fig. 12. Cut of mean heat release [$\mathrm{J\,m^{-3}\,s^{-1}}$] and iso-contours of heat release (1.79×10^8 $\mathrm{J\,m^{-3}\,s^{-1}}$, 6.46×10^8 $\mathrm{J\,m^{-3}\,s^{-1}}$). Left: PCM-2 step; Right: TFLES-2 step.

3.1. Comparison of LES combustion model

The influence of the turbulent combustion model is observed by comparing PCM-2 step (dashed curves), and TFLES-2 step (lines) with experimental data (circles).

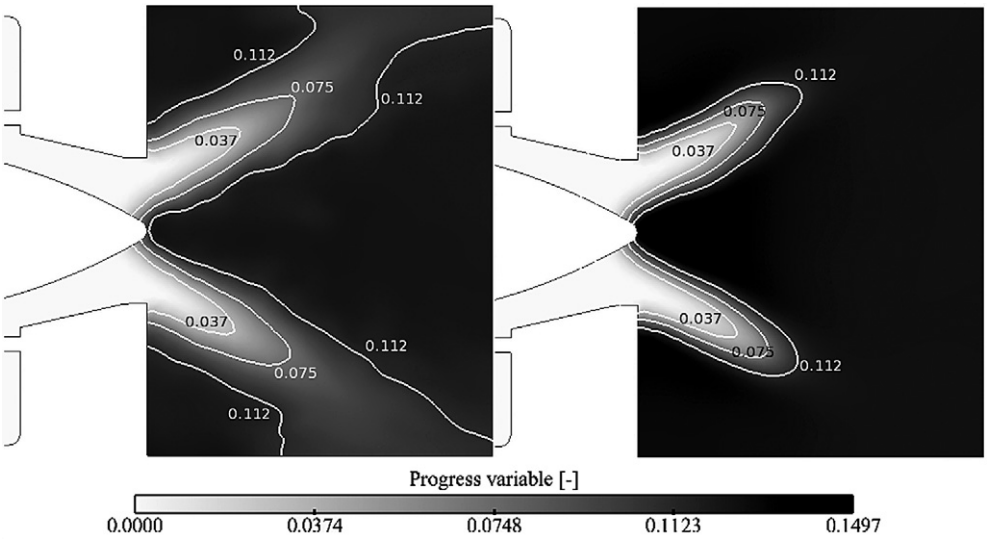

Fig. 13. Cut of mean normalized progress variable [–] and iso-contours of normalized progress variable (0.037, 0.075 and 0.112). Left: PCM-2 step; Right: TFLES-2 step.

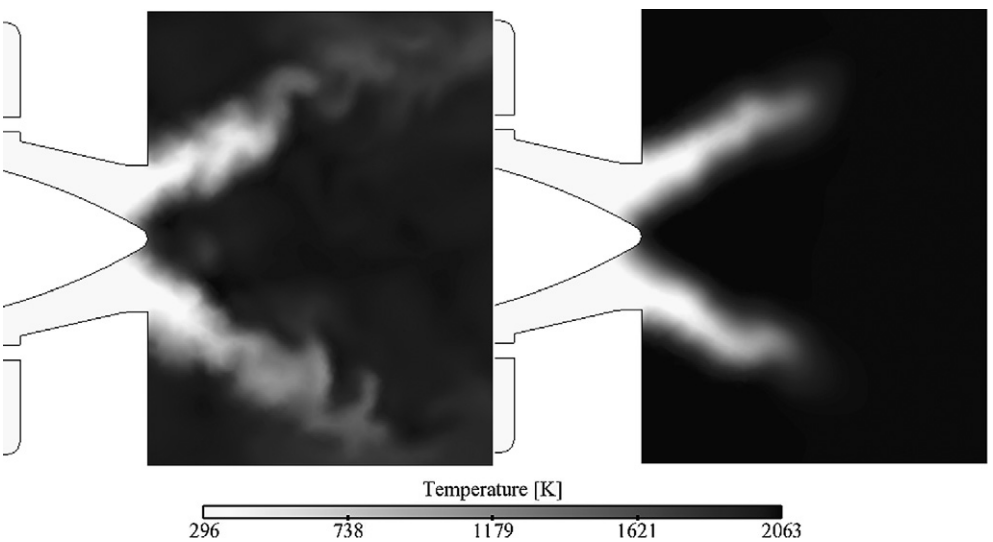

Fig. 14. Cut of instantaneous temperature [–]. Left: PCM-2 step; Right: TFLES-2 step.

For temperature profiles (Fig. 8), there is no major difference between PCM and TFLES simulations. This is the same for RMS profiles (Fig. 10), although TFLES values are always slightly smaller than PCM ones.

Concerning CO mass fraction profiles, there are some discrepancies between PCM and TFLES simulations. The main difference is that TFLES over-estimates CO mass fractions along the center-line ($r = 0$) of the domain. There is a major difference between LES and experimental data on CO mass fractions: experimental data have only two drops of CO mass fraction, whereas LES data have four. It seems natural to find four drops when displacing radially in the first measuring planes of the combustion chamber, because four flame fronts are found. Inside each of these fronts, CO is produced and almost fully consumed. The large uncertainty on CO mass fraction experimental data (between 20 and 50%, see [27]) has to be kept in mind when comparing with LES.

PCM-2 step and TFLES-2 step heat release and normalized progress variable averaged fields are compared on Figs. 12 and 13. Instantaneous temperature are compared on Fig. 14.

Heat release is compared based on an average field in Fig. 12. The TFLES flame seems to be anchored to the burner extremity while the PCM flame seems to be located inside the injector. The PCM flame seems to be larger and more diffused than the TFLES one. Two reasons could lead to this observation: either the flame is really larger (i.e. thickened), either it is less stable and moves around its mean position. This second possibility seems to be confirmed by RMS values (see Fig. 10), which are smaller for TFLES than for PCM, and by instantaneous cuts of temperature (see Fig. 14).

Concerning the averaged normalized progress variable (Fig. 13), the main difference between both cases is that the PCM flame seems to burn until it touches walls, contrary to the TFLES case that seems to respect a conical shape, classical of swirled flames [35]. This is also visible on mean and instantaneous temperature fields. There is still "fresh" gases near walls when everything is burnt in the TFLES case.

3.2. Comparison of chemical kinetics modeling

The influence of the chemical kinetic modeling is observed by comparing the PCM-2 step (dashed curves), and PCM-FPI (dotted curves) over the experimental data (circles). Temperature profiles (Fig. 8) are in good agreement, although all simulations show some difficulties to match temperature outside of the jet, near the walls. LES always over-estimates temperature of the outer recirculation zone in the first 40 mm of the chamber. It is probably due to the fact that heat losses to the combustion chamber walls are not taken into account. In the simulations, walls are considered adiabatic.

Complex chemistry reaction rates are greater than reduced kinetic schemes, since complex chemistry temperatures are always slightly greater than those of reduced chemistry (Fig. 8). Both simulations seem to over-estimate reaction rates since experimental temperatures are always over-estimated.

CO mass fraction profiles picture differences between complex and reduced chemistry. Reduced chemistry always under-estimates locally CO mass fractions, despite the fact that final mass fractions are almost the same for every simulations.

Temperature RMS profiles (Fig. 10) are very close between the PCM-2 step and PCM-FPI simulations. As expected, it is not the case for CO, since averaged CO mass fractions are greatly under-estimated in the case of the reduced kinetic scheme simulation.

4. Conclusions

This study has been motivated by the need to understand turbulent combustion models and chemical kinetic modeling effects on temperature and species mass fractions in the context of LES. A complex swirled turbulent combustor is simulated to study averaged and RMS profiles of temperature and species mass fractions. Prior to this analysis, a PDF approach turbulent model has been compared to the thickened flame model keeping the chemical scheme simple and identical in both simulations. Kinetic scheme reduction effects have then been studied.

In the case of this swirled combustor and with the perfectly premixed assumption, conclusions are as follows:

- Conclusion on chemical kinetics modeling:
  - both complex and reduced chemistry seems to over-estimate reaction rates, this point being more important for complex chemistry than for reduced chemistry;
  - complex chemistry provides better results than reduced chemistry for CO mass fractions. However, reduced chemistry is still able to predict final values of CO.
- Conclusion on turbulent combustion modeling:
  - PCM and TFLES yield very close mean results, except for CO that is over-estimated by the TFLES approach, especially along the center line of the combustion chamber;
  - The mean PCM flame is larger and more diffused than TFLES one.

This study has shown that reactive LES has good capabilities for complex combustors and that experimental profiles are well matched. It has also proved that some ameliorations could still be made. Among them, the perfectly premixed hypothesis has to be removed and heat losses at wall have to be taken into account. This is the object of future publications.

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