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Large-Eddy Simulation of a turbulent spray flame using the flamelet generated manifold approach

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Abstract

In order to meet the increasingly stringent regulations in terms of pollutant emissions adopted by ICAO-CAEP in last years, a redesign of aero-engine combustors has been required and, today, lean combustion technology can be considered as the most effective solution. In this context, common design tools and standard RANS predictive techniques are often not capable of properly characterizing combustors performances.Thus, computational techniques have been rapidly evolving towards an extensive use of Large-Eddy Simulation (LES) or hybrid RANS methods. This paper presents the numerical analysis of an experimental partially premixed flame fed by a dilute spray of acetone[1], exploiting a two-phase Eulerian-Lagrangian approach combined with the Flamelet Generated Manifold (FGM) combustion model in the context of LES techniques. All simulations have been performed with thecode Ansys Fluent 15.0.

A comparison both in non-reactive and reactive conditions of the obtained results with experimental data and conventional RANS solution has been realized in order to highlight the LES capabilities to give a new insight into the physics of reactive two-phase flows, particularly on the unsteady evolution of turbulent spray flames involving particles dispersion, evaporation and combustion.

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Keywords: Large Eddy Simulation; Spray flame; FGM; Euler-Lagrangian;

1. Introduction

With the future standards on pollutant emissions imposed by ICAO-CAEP [2], that force to a drastic reduction of current NO_x levels, lean combustion, successfully applied in heavy duty gas turbine from 20 years, will be soon adopted in aero-engines as well. However, such redesign process needs to deal with the onset of large pressure fluctuations and aeroacoustics phenomena that should be solved in order to safely implement this burning mode. In this framework, standard design tools are often not sufficientto properly characterize such devices. Thus, scale resolved and unsteady approaches are required to properly

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understand the combustor performances and to these reasons Large Eddy Simulation (LES) has undergone considerable developments. This approach has been widely applied for the numerical simulation of gaseous flames [3]leading to a strong enhancement in phenomena prediction with respect to standard steady-state approaches, while huge research efforts are still required when spray flames are considered. Indeed, all numerical models chosen to describe spray dynamics and combustion phenomena can have a strong impact both on CPU effort and accuracy of the whole simulation. Hence, detailed preliminary studies, even on experimental academic test case, are required in order to assess the involved models.

In this work, LES simulations of a piloted round-jet test flame [1]fed by a spray of acetone under non-reactive and reactive conditions are reported and compared with the available experimental data. A detailed comparison also with RANS simulations on the same case is shown in order to highlight the improvements that can be obtained with scale-resolved approaches. Code Ansys Fluent 15.0 is used in all simulations.

2. Mathematical formulation

2.1. *LES modelling and interaction of gaseous and dispersed phase*

In LES modelling of two phase flows, a density weighted localized spatial filter is applied to Navier-Stokes equations[4].In the equation for filtered species, the unclosed reaction rates must be modelled and they will be analyzed in Section 2.2. At the same time also the unclosed sub-grid stress tensor appears and in this work a dynamic Smagorinsky-Lilly model has been exploited [5].

For the dispersed phase description a Lagrangian formulation has been adopted. Such approach is suitable when no primary break-up occurs and the spray can be described with a dilute assumption and in this test case such assumptions are well satisfied due to the low values of liquid volume fraction and Weber number, as also discussed in[6].Models for droplet motion, evaporation and heat transfer are needed to obtain spray distribution and provide source terms of mass, momentum and energy to continuous phase. In this work, for the liquid momentum equation, buoyancy and gravity effects have been neglected and the drag coefficient has been evaluated through the hypothesis of spherical not deformable shape as provided in [7]. Such hypothesis is justified by low values of Weber and Ohnesorge number in the entire domain that lead also toneglect secondary break-up effects.Furthermore, during their motion, droplets interact with fluid turbulent structures modifying their trajectory in a process usually referred to as turbulent dispersion. In particular, even though sufficiently small particles normally tend to follow the fluid, larger droplets, due to their higher inertia, generate wake structures and velocity gradients that must be considered. In present LES computations, in order to add these contributions, a stochasticapproach, known as Discrete Random Walk model, has been exploited.The reader interested in this topic is addressed to reference [8]where such model is presented in detail.

Moreover, for the evaporation modelling a uniform temperature model has been considered where the integration of convection contribution on the mass transfer is included exploiting the formulation derived in [9]. Uniform temperature assumption is commonly applied in discrete phase modelling due to the small particles diameter that allows neglecting the temperature distribution inside the droplet. Properties of gaseous phase around each droplet have been evaluated using the one-third rule[10], while for the liquid fuel the formulation of [11]has been exploited.

2.2. Combustion model

As discussed in section 2.1, a set of unclosed reaction rates in species conservation equation appears. It should be considered that in LES approaches, combustion model has a higher impact than the sub-grid

stress closure since all reaction rate effects are accounted in the sub-grid scale components and any part of its contribution is directly solved [4]. Moreover, in aero-engine combustors, due to the use of liquid fuels, flames present a partially-premixed nature that should be correctly modelled by the chosen combustion model.

In this work, Flamelet Generated Manifold (FGM) approach [12]has been exploited where a set of 1D laminar flames is used to construct a manifold in the composition space that is used to calculate the evolution of the reactive phenomena. Hence, in the manifold generation, the flamelet equations are solved for a set of combinations of normalized progress variable ($c=Y_c/Y_{c,eq}$) and mixture fraction Z where the un-normalized $Y_c$has been evaluated in this study as:

$$Y_c = \frac{Y_{CO\,2}}{M_{CO\,2}} + \frac{Y_{CO}}{M_{CO}} + \frac{Y_{H20}}{M_{H20}} + \frac{Y_{H2}}{M_{H2}} \quad (1)$$

including$CO$and H_2 that may have a strong impact in a rich mixture combustion. As suggested in[6], a diffusive flamelet behavior has been considered and a detailed reaction mechanism for acetone as provided in [13] with 84 species and 409 reactions has been exploited. Furthermore, the interaction between flame and turbulent variables has been accounted through a Presumed Probability Density Function approach[6][4]. In order to include heat losses, due to spray evaporation, an extra dimension due to the filtered enthalpy gain/loss has been added to the tables, while radiative effects have been neglected.

3. Experimental set-up and numerical details

Two phase Large Eddy Simulations of a series of spray of acetone both under non-reactive and reactive conditions have been performed using the experimental results reported in [1]. The experimental apparatus consists of a jet surrounded by a pilot and an annular primary co-flow, where the liquid fuel is released upstream of the jet exit plane by an ultrasonic nebulizer and the generated droplets are carried in the feeding pipe. In reactingconditions a pilot flame fed by a stoichiometric mixture of acetylene, hydrogen and air is used to stabilize the flame (see Figure 1a).

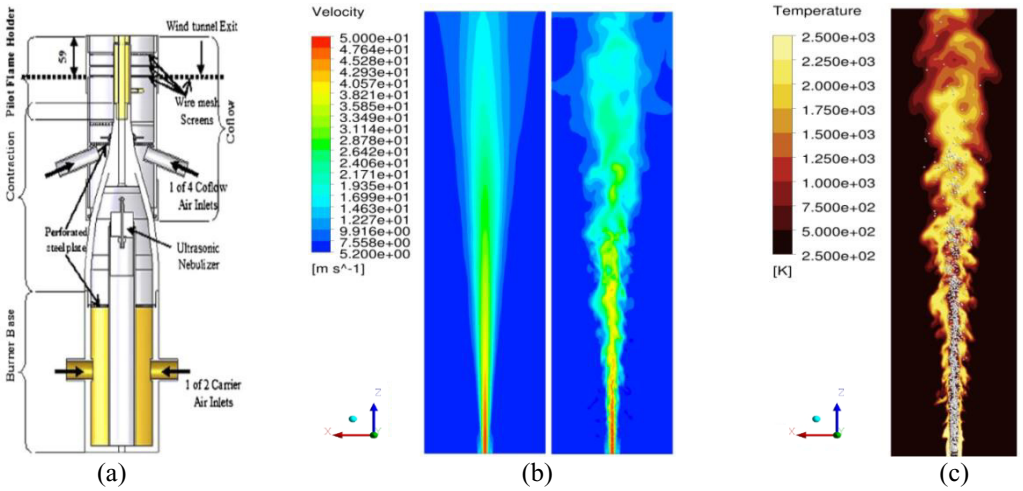

Figure 1:Experimental set-up (a), contours of mean and instantaneous velocity (b), contour of instantaneous temperature with liquid phase evolution (c).

A detailed description of the experimental setup used for the generation and collection of the experimental data can be found in [1].

Several cases at atmospheric pressure are reported with various global equivalence ratio and in this work test point described in Table 1has been considered.

The computational domain exploited in LES calculation takes the region downstream of the exit plane with a computational setup similarly to the one used in[6]. The computational mesh (a structured hexahedralmesh) represents a 360 degrees cylindrical domain and has been generated with Ansys Fluent Meshing 15.0 with a minimum size of 0.4 mm. The extension of the computationaldomain in radial direction is about $8d_{jet}$ and $75d_{jet}$in the axial one to reduce the influence of boundary conditions.

Mesh resolution has been verified both in reactive and non-reactive conditions following [14]with a definition of the turbulent kinetic energy taken from [15]. Hence, it has been possible to verify that for all the reported simulations more than 80% of the turbulent kinetic energy is resolved with the adopted computational domain.

For non-reactive test conditions, considering a flow-through time around 0.2s, 22000 time steps were performed in order to flush-out boundary conditions and allow the flow-field to develop. Statistics were then gathered over more than one flow-through time. The same set-up has been exploited also for the reactive test case, where, due to the combustion process, the flow-through time is around 0.1s. All comparisons here shown have been realized using mean quantity values.

As already mentioned, a set of preliminary RANS simulations has been realized and, in order to decrease the computational effort, a sector of 15 degrees has been realized with the same geometrical features.In LES calculations second order schemes for all the resolved quantities havebeen used to minimize numerical dissipation.

Applied boundary conditions follow a classical scheme for compressible flows with the experimental mass flow specified at the inlet boundary and a static pressure prescribed at outlet. Mass flow profile and turbulent quantities distribution at the jet inlet patch has been derived from[1]. For LES calculations spectral method [16]has been activated in order to calculate instantaneous velocities.Finally, spray boundary conditions have been imposed injectingsets of parcels with experimental characteristics at several radial and tangential locations at domain inlet. Indeed,dropletsproperties, such as diameter, velocity and mass fluxhave been extrapolated from the experimental measurements at $x/d_{jet}=0.3$ plane and for each position ten parcels, corresponding to ten equispaced diameter classes ranging from 0 μm to 100 μm, have been injected. Moreover, in order to reduce the negative effects of a discrete spray injection, particle staggering has been considered.

Table 1. Experimental data of chosentest point[1].

U_{jet} (m/s)	$\dot{m}_{air}$ (kg/s)	$\dot{m}_{fuel}$ (kg/s)	ϕ	Re_{jet}	T_{jet}(K)
36	3.75×10^{-3}	1.25×10^{-3}	3.2	31700	300

4. Results and discussion

Firstly, in order to verify that the chosen numerical domain and the sub-grid model are able to properly describe the turbulent flow-field and its interaction with the liquid phase, non-reactive test conditions have been considered. In Figure 1b a qualitative comparison between instantaneous and mean velocity fields is reported. Figure 2 shows the resulting comparison amon LES, RANS and experimental data at three cross sections in terms of axial velocity (U_{ax}), axial velocity standard deviation (U_{ax}'), mean droplet diameter (D_{10}) and volumetric flux (V_l).

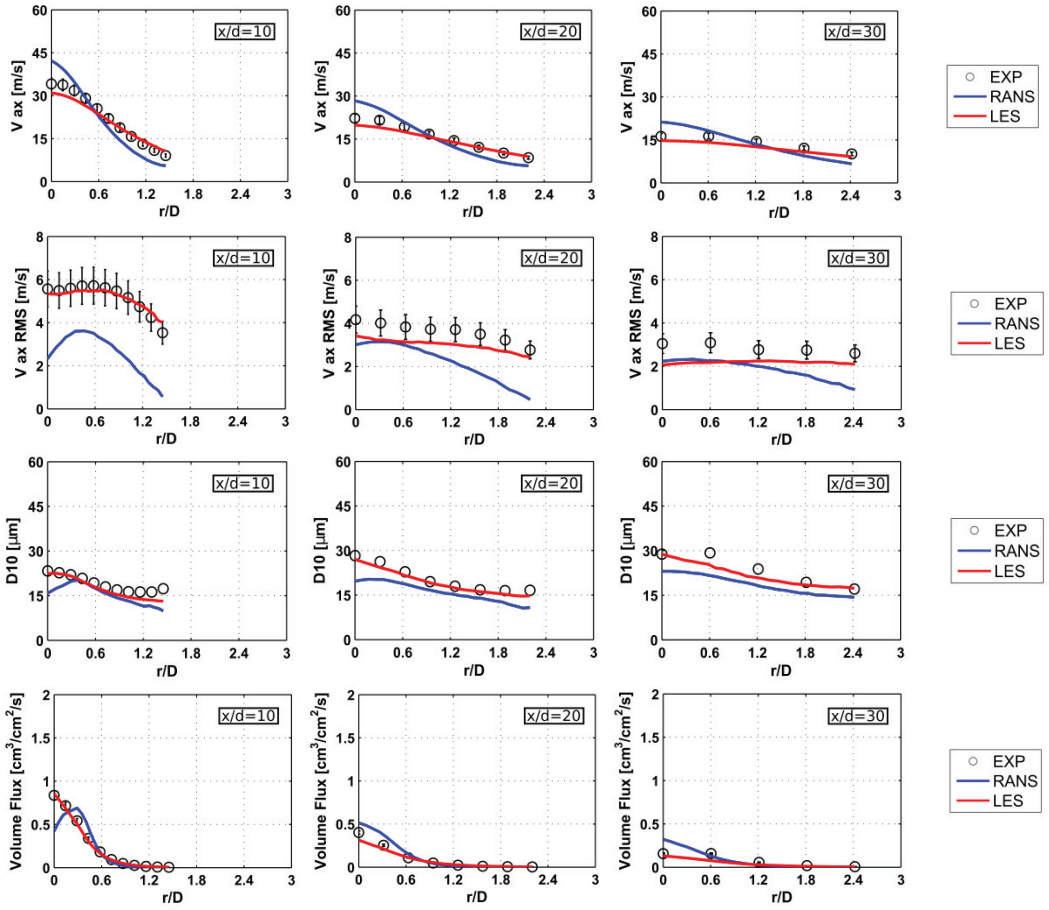

Figure 2:Radial profiles of droplet mean axial velocity, axial velocity fluctuation, droplet diameter and volume flux at different distances from the nozzle exit plane in non-reactive test conditions.

Experimental data also for the radial velocity would be available but in the chosen test conditions the axial component is prevailing and it has been considered for the assessment of the numerical set-up. In this work, the volumetric flux has been defined as:

$$V_l = \frac{\alpha_l \|\overrightarrow{U_l}\|}{A_p} \tag{2}$$

whereA_p is a passage area for each droplet and α_l is the liquid volume fraction.

A general good agreement between numerical and experimental data can be observed. The radial evolution of mean axial velocity is well predicted both with RANS and LES approaches, but its fluctuation is completely underestimated in steady simulations. This leads in LES calculations to a more physical behaviourof the spray that is properly interacting with the continuous phase turbulent fields. Indeed, with respect to RANS, both the evolution of mean droplet diameter and liquid volume flux, which is a reliable indicator of evaporation rate mainly in such non-reactive test conditions, are well calculated and RANS inconsistencies in proximity of the axis are completely avoided.

Hence, this preliminary assessment leads to the first conclusion that, with the same physical properties for liquid, LES, solving larger turbulent structures, is able to better reproduce the evolution of the spray and its distribution inside the numerical domain.

Considering the reactive test conditions, Figure 1c shows the evolution of the instantaneous temperature together with the liquid phase tracking. The quantitative comparisonof its mean value with RANS and experimental results is reported in Figure 3.

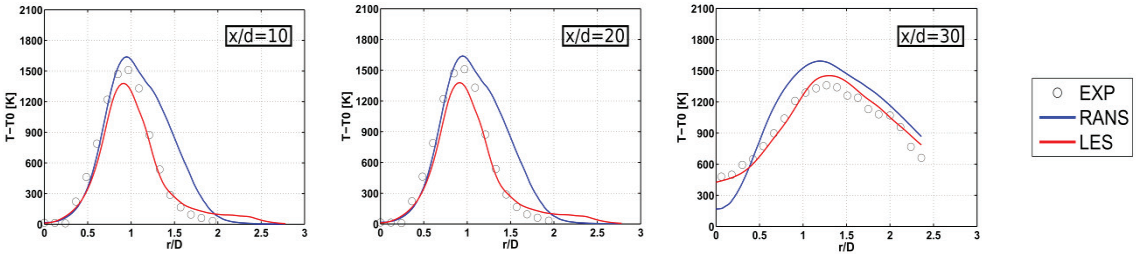

Figure3: Radial profiles of the excess temperature at different distances from the nozzle exit plane in reactive test conditions.

As in non-reactive conditions, LES simulation leads to a more physical evaluation ofsuch variable except for the maximum value mainly at x/d_{jet}=20. Such discrepancy can be justified considering that in this study the effects of spray in flamelet generation have been neglected and that probably in such region a diffusive flamelet approach is not correct due to the local lean value of equivalence ratio.At the same time, at x/d_{jet}=30 LES results are correctly reproducing the experimental behavior while RANS is completely wrong. Such physical behaviouris again confirmed by the other spray quantities as reported in Figure 4.

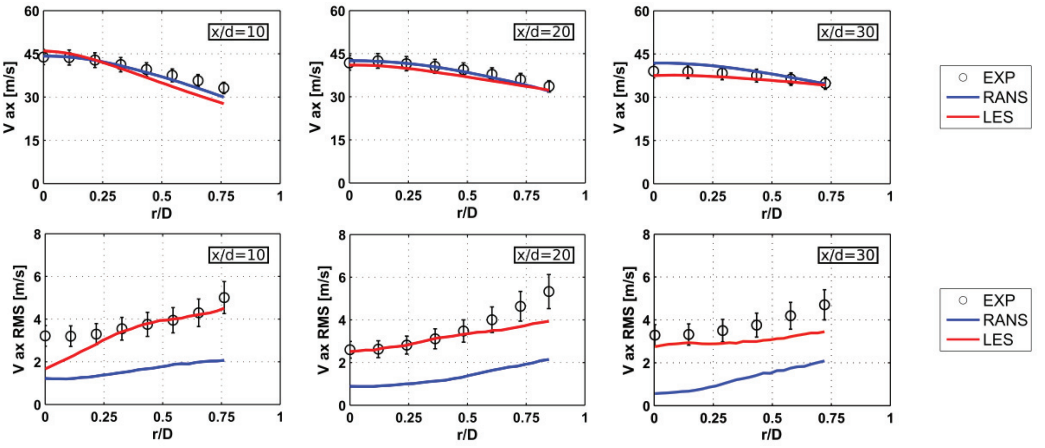

Figure 4: Radial profiles of axial velocity magnitude and its fluctuation at different distances from the nozzle exit plane in reactive test conditions.

5. Conclusions

In this work, LES calculations of a spray of acetone under reactive and non-reactive conditions have been considered. The comparisonbetween experimental and RANS results show that LES is able to better

estimate the interaction between the spray and the turbulent field leading to a more accurate estimation of the analyzed reactive process.

Acknowledgements

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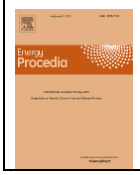

Biography

Stefano Puggelli is a Ph.D. student of the Department of Industrial Engineering at the University of Florence. His research activities are mainly focused on the numerical modelling of turbulent two phase combustion with unsteady and scale resolved approaches.