Assessment of a numerical procedure for scale resolved simulations of turbulent spray flames

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Abstract
The present paper consists in a collection of CFD simulations with increasing geometrical complexity aimed to investigate phenomena occurring in turbulent spray flames and to develop a reliable numerical procedure useful in the design of aero-engine combustors. Scale Resolved Simulations (SRSs) were performed using Flamelet Generated Manifold (FGM) and Eddy Dissipation Model (EDM) for combustion modelling and an Eulerian-Lagrangian approach for droplet evolution.
Results highlight outstanding enhancements in the prediction of spray flame behavior using SRSs in place of classical RANS approaches.

Introduction
With the future standards on pollutant emissions of civil aero-engines required by ICAO-CAEP, lean burn technology could become in the next years an effective solution for aero-engines combustors. However, instability issues should be solved in order to safely implement this burning mode. In this framework, standard RANS simulations are often not sufficient to properly characterize such devices. Thus, scale resolved approaches are required to properly understand the combustor performances. Several works can be found in literature about SRSs of gaseous flames, whereas such approaches are still not completely assessed for spray flames. For this reason, numerical models for spray dynamics and combustion processes should be validated on test cases gradually closer to real aero-engine combustors in terms of geometries and operating conditions.
In the present work three test cases characterized by increasing complexity were investigated in the Large-Eddy Simulation (LES) and Scale-Adaptive Simulation (SAS) frameworks exploiting an Eulerian-Lagrangian approach for spray modelling, combined with Flamelet Generated Manifold (FGM) or Eddy Dissipation Model (EDM) for reaction modelling. Obtained results were compared against the available experimental data and steady state solutions. All the simulations were performed using the commercial code ANSYS Fluent.

Numerical modelling
In the present work the analysis has been focused on combustion approaches and therefore all the reported simulations have been realized employing a well-established Lagrangian formulation for liquid phase modelling.
In terms of combustion modelling, two different approaches like Eddy Dissipation

Model (EDM) and Flamelet Generated Manifold (FGM) have been employed and compared during this work. EDM, which computes turbulent reaction rates relying on high Damkohler number hypothesis, has been successfully applied in the simulation of a wide range of turbulent spray flames but, since it employs global reaction mechanisms (i.e. 1-2 steps), it cannot be used to represent some local flame characteristics (i.e. flame extinction or pollutant emissions). On the other hand, FGM is based on a detailed description of the kinetic mechanisms and, using a pre-computed laminar solution weighted through a pre-defined probability density function, it proved to accurately describe the flame evolution taking into account local finite rate effects.

Experimental test cases

In this section the three investigated test cases are briefly described.

In Figure 1(a) a sketch of the so-called Sydney Spray Burner is reported. It consists of a jet surrounded by a pilot and an annular primary co-flow. The spray of acetone is released upstream of the jet exit plane by an ultrasonic nebulizer and the generated droplets are carried in the feeding pipe [1].

In Figure 1(b) the swirl stabilized spray flame experimentally investigated by Sheen in [2] is shown. The chosen test case consists of an annular air channel fed by a single axial swirler that ends in a tubular liner. A pressure atomizer, located at the center of the liner inlet plane, injects liquid kerosene, generating a hollow cone spray.

In Figure 1(c) is shown the DLR Generic Single Sector Combustor developed in the framework of the TIMECOP-AE Project and designed to represents an aero-engine lean burn [3]. It is characterized by an upstream cylindrical feeding plenum and a square-section combustion chamber. The burner is equipped with a co-

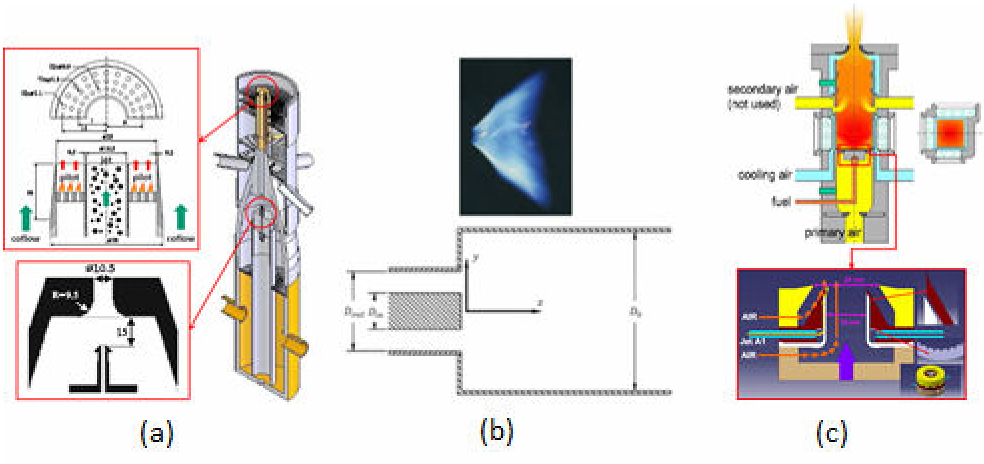

Figure 1. Sketch of the investigated test cases

rotating double radial swirler with a pre-filming air blast atomizer that injects kerosene fuel. It is worth mentioning that previous burners operate at ambient pressure, while this one at a pressure of 4 bar.

Numerical Setup

The main features of the numerical setup are here reported. In all the simulations no radiation model and heat transfer at wall boundaries were included. Velocity and pressure conditions were imposed respectively at inlet and outlet boundaries, such as to respect the experimental flow rate and profiles. In LES framework a dynamic Smagorinsky-Lilly model was exploited to close sub-grid terms. On the other hand, in order to properly predict spray evolution Discrete Random Walk (DRW) for turbulent dispersion, Taylor Analogy Breakup (TAB) model for secondary breakup and Uniform Temperature model for liquid evaporation were included. Clearly, different injection strategies were used in the three test cases. In Sydney Spray Burner parcels are injected at the jet exit plane following experimental distribution and velocities. Calculations of the other test cases, instead, assume a Rosin-Rammler distribution and employ a cone injection with parameters (cone angle α, Sauter Mean Diameter SMD and velocities) obtained by means of empirical correlation and trial-and-error procedures because of the lack of experimental data. In Sheen Burner parcels are injected at injector position while in DLR combustor injection at lip is required to avoid film modelling.

Finally, concerning FGM model, diffusive flamelets have been exploited in Sydney and Sheen burners for the PDF-table generation, while premixed flamelets were used in DLR combustor.

Results

Sydney Spray Burner, widely investigated in literature from a numerical point of view, allows to point out the capability of Scale-Resolved Simulations in predicting the interactions between the two phases, focusing especially on spray turbulent dispersion phenomenon. LES calculations lead to a more physical behavior of the spray that is properly interacting with the continuous phase turbulent field [4].

Consequently, droplets velocities, diameters and the liquid volume flux are well predicted. Such improvements become more important in reactive conditions because of the strong interaction between flame, turbulence and spray, leading to a better prediction of temperature field in LES computation as reported in Figure 2.

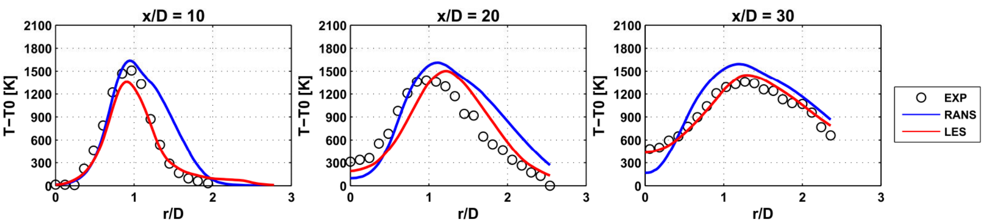

Figure 2. Temperature radial distribution of Sydney Spray Burner reactive case

A good response of the FGM model was highlighted by Sydney Burner, at least for the simulated test point. However, in order to deeply investigate the capabilities of FGM combustion model in aero-engine applications, more representative test cases with measurements of typical reactive quantities (i.e. temperature, its fluctuations and pollutant emissions) has been considered. To this end, Sheen Burner is a valuable choice. As shown in Figure 3, in this test case velocity fields of RANS

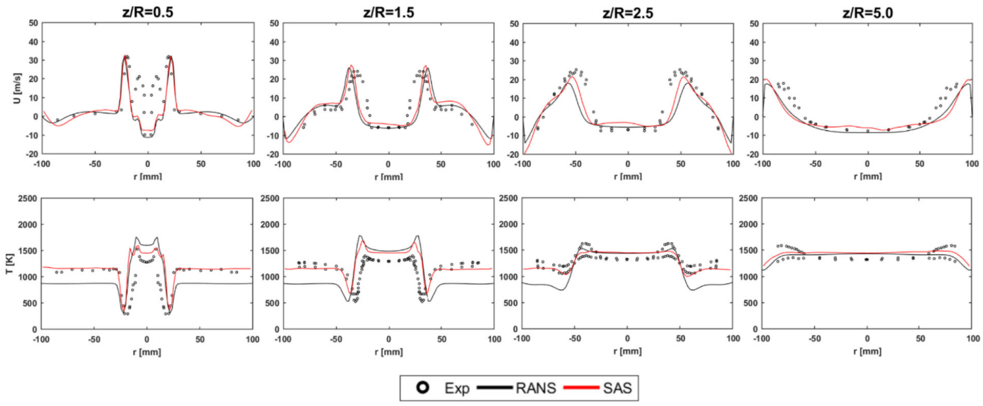

Figure 3. Radial profiles of axial velocity (top) and temperature (bottom) for Sheen Burner

and SAS simulations seem very similar and in good agreement with measurements, except for the opening angle that is slightly overestimated. Indeed, even if some major turbulent structures are caught in the near injector region by scale resolved approach, the swirling flow is qualitatively coherent as in RANS simulations, as shown in Figure 4.

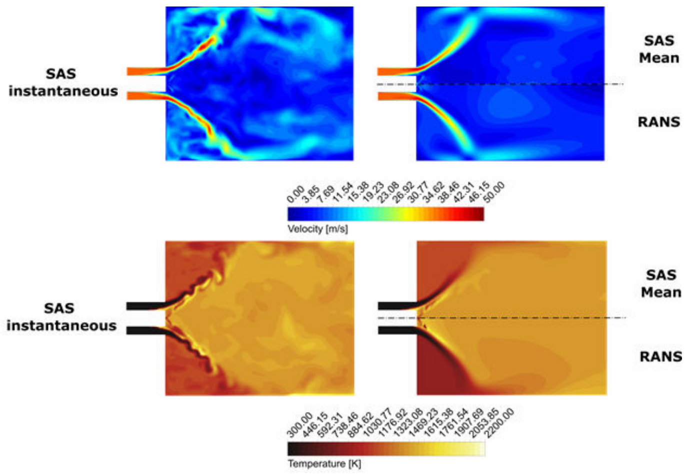

Figure 4. Contours of velocity (top) and temperature (bottom) fields of RANS and SAS simulations of the Sheen burner test case

However, a more intense corner vortex region, in addition to a more physical prediction of the mixing of vapor fuel and the turbulent dispersion of spray typical of unsteady simulations, leads to a higher temperature in corner vortex zones for SAS calculations leading to recover experimental trends.

The above numerical tools were finally tested on the DLR Generic Single Sector Combustor [5]. An isothermal test point has been used to show again that Scale Resolved Simulations (SAS and LES) are strictly required when the complexity and anisotropy of the turbulent flow field dramatically increase, leading to a more physical prediction of spray evolution and turbulent dispersion [5].

Then, a first set of reactive simulations were performed using spray boundary conditions provided by Jones et al. [6] (SMD=6 µm, α=160°). Figure 5 shows the instantaneous and mean temperature fields obtained with scale resolved simulations with different mesh sizes. Moving from SAS to LES and from coarse

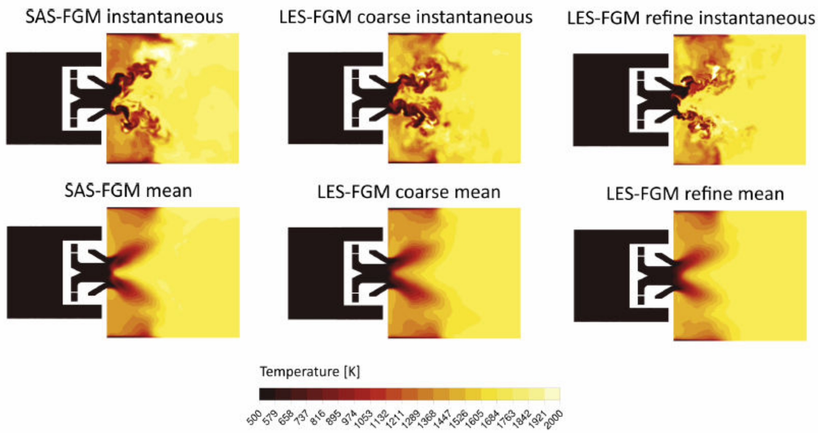

Figure 5. Contour of temperature field for simulations of DLR combustor

to fine mesh, turbulent resolved scales become smaller and smaller leading to a more physical prediction of instantaneous mixing between spray and swirled flow.

Considering mean temperature profiles experimentally observed distinct lobes at high temperature are not properly reproduced exploiting FGM model. Hence, an EDM model was then employed in SAS framework using spray BCs reported in [6] and a new set derived from available experimental correlations for prefilmer atomizers (SMD=30 µm, α=20°). EDM results, shown in Figure 6, highlight the presence of two distinct lobes at high temperature similar to the ones reported in the experimental map. Moreover, simulations with the new set of spray BCs show an overall good agreement with experimental data in terms of spray mean velocity and particle diameters. Such an improvement obtained thanks to the EDM model could be ascribed considering the premixed asymptotic flame behavior, supposed in FGM flamelet generation, that is not completely representative for the flame under investigation.

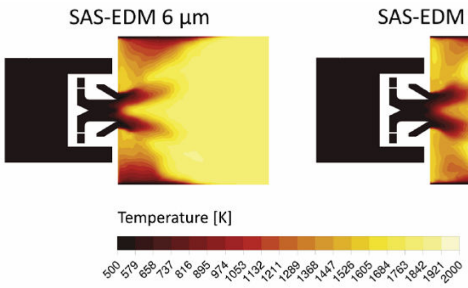

Figure 6. Contour of temperature field for SAS-EDM simulations of DLR combustor

Nomenclature

SMD	Sauter mean diameter
α	Cone angle
LES	Large Eddy Simulation
SAS	Scale Adaptive Simulation
RANS	Reynolds Averaged Navier Stokes
EDM	Eddy Dissipation Model
FGM	Flamelet Generated Manifold
BC	Boundary Condition

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