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Large Eddy Simulations (LES) towards a Comprehensive Understanding of Ducted Fuel Injection Concept in Non-Reacting Conditions

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Abstract. The diesel combustion research is increasingly focused on Ducted Fuel Injection (DFI), a promising concept to abate engine-out soot emissions in Compression-Ignition engines. A large set of experiments and numerical simulations, at medium-low computational cost, showed that the duct adoption in front of the injector nozzle activates several soot mitigation mechanisms, leading to quasi-zero soot formation in several engine-like operating conditions. However, although the simplified CFD modelling so far played a crucial role for the preliminary understanding of DFI technology, a more accurate turbulence description approach, combined with a large set of numerical experiments for statistical purposes, is of paramount importance for a robust knowledge on the DFI physical behavior.
In this context, the present work exploits the potential of Large Eddy Simulations (LES) to analyze the non-reacting spray of DFI configuration compared with the unconstrained spray. For this purpose, a previously developed spray model, calibrated and validated in the RANS framework against an extensive amount of experimental data related to both free spray and DFI, has been employed. This high-fidelity simulation model has been adapted for LES, firstly selecting the best grid settings, and then carrying out several numerical experiments for both spray configurations until achieving a satisfying statistical convergence. With this aim, the number of independent samples for the averaging procedure has been increased exploiting the axial symmetry characteristics of the present case study. The reliability of this methodology has been herein proven, highlighting an impressive runtime saving without any remarkable worsening of the accuracy level.
Thanks to this approach, a detailed description of the main DFI-enabled soot mitigation mechanisms has been achieved, bridging the still open knowledge gap in the physical understanding of the impact of spray-duct interaction.

1. Introduction

The urgency of keeping air quality under control and limiting the global warming due to the anthropogenic greenhouse gas emissions are pushing a substantial portion of the internal combustion engines research to find new strategies to abate soot (i.e., black carbon) emissions from diesel combustion.

A particularly interesting solution is Ducted Fuel Injection (DFI), a hardware-related concept currently under investigation in several research groups across the world. The DFI, conceived by Mueller et al. [1], means assembling a small cylindrical pipe coaxially, some distance downstream, to the injector nozzle, aiming at improving the mixture preparation upstream of the autoignition zone. A dramatic soot reduction through DFI, compared to the conventional free spray, has been demonstrated in combustion studies, performed both in Constant-Volume Vessel (CVV) [1,2] and in optically accessible Compression-Ignition (CI) engine [3]. However, a clear and generally accepted explanation of the DFI soot mitigation mechanisms still misses, despite the large number of physics-oriented studies available in literature in both non-reacting and reacting conditions, using experiments and CFD. This comprehensive understanding is of paramount importance in making DFI technology suitable for a large and complex range of operating conditions, such as the one characterizing a typical CI engine map, as well as in supporting from a geometry optimization and assembly perspective.

In light of this, the purpose of the herein work is to analyze the non-reacting spray of DFI configuration compared with the unconstrained spray to a deeper level, involving 3D-CFD with a high-fidelity spray model and an accurate turbulence modelling approach like Large Eddy Simulation (LES), adopting a grid size able to capture very small turbulent eddies and performing several numerical experiments until achieving a satisfying statistical convergence. The large computational cost associated with this approach has been significantly reduced though the method suggested in [4],

thus increasing the number of independent samples by exploiting the axial symmetry characteristics of the present case study. The reliability of this methodology has been herein proven for the DFI case, before its employment for the detailed physical analysis, which is the main object of this research.

2. Methodology

2.1. Case Study

The case study considered for this LES analysis was presented in [5,6], where a free spray configuration was compared with DFI concept in CVV, in both non-reacting and reacting conditions, using a prototype single-hole Common Rail injector with a 0.180 mm nozzle diameter. Both spray configurations are herein considered, under the non-reacting operating conditions summarized in Table 1.

Table 1. Operating conditions

Rail pressure	1200 bar
Injection duration	1.5 ms
Vessel pressure	20 bar
Vessel temperature	773 K

As far as the DFI configuration is concerned, the duct features a diameter of 2 mm, a length of 14 mm and a stand-off distance (i.e., the gap between duct inlet and injector nozzle) of 2 mm.

2.2. 3D-CFD Simulation Setup

The 3D-CFD analysis was carried out by means of the commercially available software CONVERGE CFD V3.0.14 [7]. The spray model was developed in the RANS framework [5,6,8], extensively validated against experimental data in both free spray and DFI configuration. For the turbulence modelling, the LES approach was employed, allowing for direct resolution of the largest turbulent scales. The one-equation dynamic structure model was used for the sub-grid scale [9].

The computational domain was meshed with a cartesian grid by means of the CONVERGE CFD patented cut-cell technique, reaching a minimum grid size of 31.25 µm in the most critical areas through the Adaptive Mesh Refinement (AMR) tool. This final value was the result of a grid sensitivity analysis, aiming at a high-quality LES resolution in the whole domain of interest for both configurations. In particular, a minimum target of 80% of resolved turbulent structures was achieved, as suggested by [10,11]. This minimum grid size, relatively low if compared with most of the LES spray simulations available in literature, was especially required for the DFI case, to obtain a good description of the inflow at the duct inlet and outflow at duct outlet, where the flow detachment plays a key role. At the duct wall, a Near Wall Modelling (NWM) approach was used, adopting the wall function developed by Werner and Wengle [12] and adopting a 1-layer inlaid mesh at the inner wall, whose extrusion dimension (62.5 µm) was accurately calibrated in order to match the y+ criteria. The choice of a NWM approach was determined by the prohibitive computational cost needed to resolve the boundary layer with a LES turbulence model at high Reynolds number conditions.

2.3. Ensemble Average Method

For the herein study, a runtime saving methodology to ensemble average several axial symmetric LES spray simulations was employed. As stated by Farrace et al. [4], considering a cylindrical test vessel equipped by a single-hole injector coaxial to the cylinder axis, the conventional approach (herein named *standard approach*) is to obtain a certain number of statical samples (N) by running S=N simulations, varying either initial conditions or random seed parameters. Nevertheless, considering a certain number (M) of semi-slices parallel to the spray axis, and by assuming that each semi-slice behaves as a different numerical experiment, if statistical independency is ensured by a sufficient angular distance among semi-slices, the same number of statistical samples (N) can be achieved by S=N/M simulations. This approach (herein named *multi-slice approach*) enables a M-fold reduction in computational costs with the drawback of limiting results to a 2D representation. For the sake of clarity, a schematic representing the two considered ensemble average methods is reported in Fig. 1, considering M=4 for the multi-slice approach.
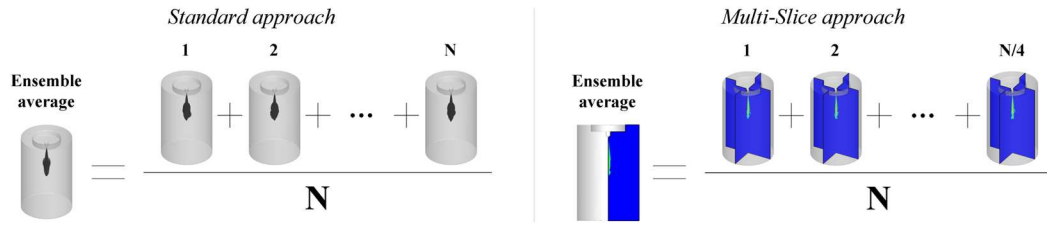
Fig. 1. Sketch of the ensemble average methods at equal number of samples

The first step of this analysis was the assessment of the abovementioned multi-slice approach, especially for the DFI configuration, considering the ensemble average among 20 different samples. However, it is not herein reported for the sake of brevity. Since this methodology resulted to be reliable and the number of samples sufficient, the multi-slice approach was adopted, and the same settings were maintained for the subsequent physical analysis.

3. Results

In Fig. 2, the resolved Turbulent Kinetic Energy (TKE) distribution on a longitudinal semi-slice is reported for both free spray and DFI configurations at four different time instants during the injection event. The resolved TKE, computed starting from the root mean square of the average velocity fluctuations component [10], can be used as turbulent mixing index, as carried out in [5,6,8].

At each time step, it can be observed that the high turbulence values for the free spray case are strongly localized in the spray tip, while for the DFI are widely distributed on the whole spray plume after the duct outlet. Hence, starting from the duct outlet, a larger and longer area (up to the spray tip) characterized by high TKE values is present for the DFI. This is caused by the flow detachment at the duct outlet, where the spray is suddenly no more guided by the duct wall and strong velocity, density and concentration gradients appear. Focusing on the duct wall, a small high-mixing region can be detected, which was identified as a first stage turbulent mixing in previous studies [6].

More in general, the energy cascade seems spatially more advanced due to the duct adoption, shifting back TKE values higher than 2000 m2/s2 of 10-20 mm. Even though the maximum value in the domain at equal time step can be higher for the free spray, it is more important that DFI enables a wider and more advanced turbulent mixing, especially considering the limited dimension of a combustion chamber and the necessity to reduce the fuel-to-air ratio before the Lift-Off Length (which is even extended by the duct adoption [1,2]).
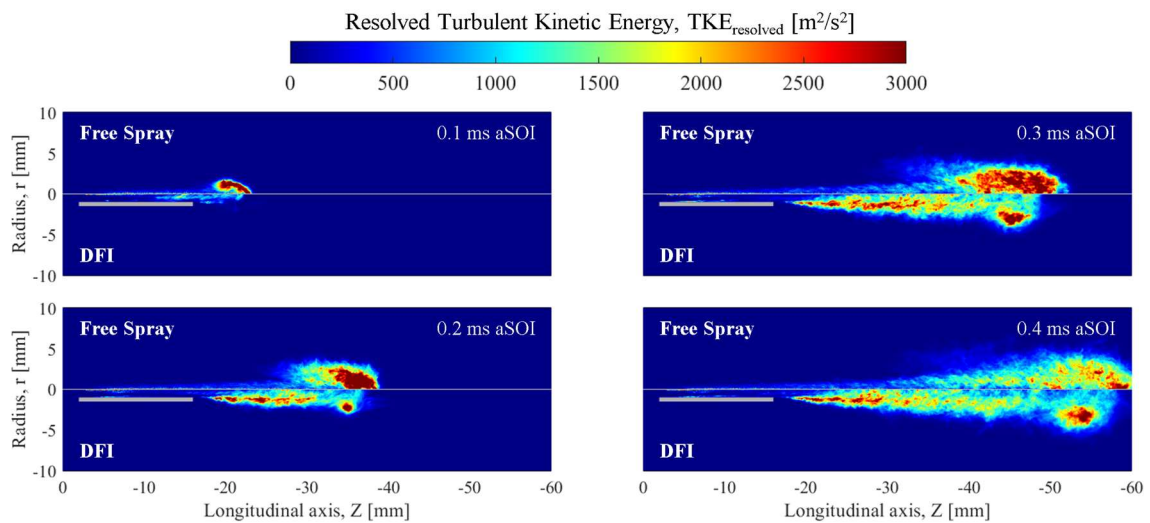

Fig. 2. Resolved Turbulent Kinetic Energy distribution on a longitudinal semi-slice for both free spray (top side) and DFI (bottom side) at four time instants during the injection event

In Fig. 3, the equivalence ratio (ϕ) distribution on a longitudinal semi-slice is reported for both free spray and DFI configurations at 0.3 ms after Start of Injection (aSOI). In this case, for a better visualization of the formation of vortices, also the outcome from a randomly selected realization is reported (left) together with the ensemble average (right).

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The free spray is characterized by a rich central core which is broken and mixed with the available air at about 40 mm from the injector nozzle on average; namely, when the high turbulent mixing is present according to Fig. 2. In the DFI case, no central rich core is present, while a high ϕ region exits the duct close to the wall, due to the inhibited contact with air. This region is rapidly broken by the high second stage turbulent mixing (Fig. 2), leading to a leaner mixture about 20 mm in advance with respect to the free spray on average. Focusing on the single realization, this rich core breakage is associated to the formation of small vortices immediately after the duct outlet. To reach similar turbulent eddy dimensions in the free spray case, additional 15-20 mm distance is needed.

It is noteworthy that also the shape of the spray plume is drastically changed by the duct adoption. In fact, a more compact mushroom shaped head is present for DFI, as already observed in [13].
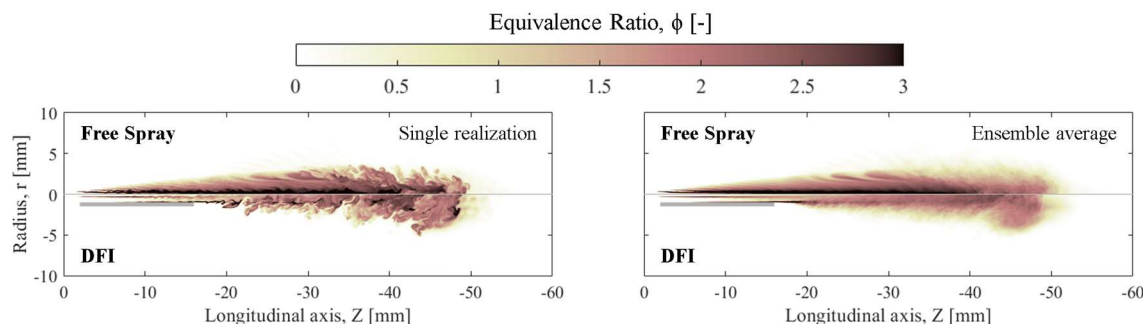

Fig. 3. Equivalence ratio distribution on a longitudinal semi-slice for both free spray (top side) and DFI (bottom side) at 0.3 ms aSOI. Results for both a randomly selected realization (left) and the ensemble average (right).

Conclusions

A 3D-CFD analysis was carried out to analyze Ducted Fuel Injection (DFI) physical behavior compared to the free spray case in non-reacting condition. The Large Eddy Simulation (LES) turbulence model, a highly refined computational grid, and a large set of numerical experiments enabling statistical analysis have been employed to bridge the still open knowledge gap about the impact of spray-duct interaction. The computation of resolved Turbulent Kinetic Energy (TKE), the definition of high turbulent mixing regions in terms of values and location, the observation of the rich cores, and the study of small and large vortices formation allowed improving the understanding on this promising technology for low-soot diesel combustion.

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