POLITECNICO
MILANO 1863

SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Executive Summary of the Thesis

CFD analysis of Ducted Injection in a Constant Volume Vessel

Laurea Magistrale in Mechanical Engineering - Ingegneria Meccanica

Author: Simone Pavesi, Gabriele Sacchetti

Advisor: Prof. Gianluca D'Errico

Co-advisor: Andrea Schirru

Academic year: 2022-2023

1. Introduction

Soot deriving from combustion processes is a significant pollutant driving the most significant health problems and the second most critical climate-forcing species after carbon dioxide CO_2. The necessity of lowering the emissions to avoid harmful consequences on the environment is also underlined by its regulations which are becoming increasingly stringent, posing great challenges to diesel engine technology. By virtue of that, a new solution termed Ducted Fuel Injection (DFI), which acts directly on the combustion process, is proposed for achieving an enhanced charge-gas mixing upstream of the lift-off length by using a small tube placed at a short distance downstream of the injector orifice.
The DFI technology results in an interesting technology for soot reduction since it brings to advantages like:

- To increase the velocity gradients responsible for the turbulent mixing within the spray, reducing the equivalence ratios of the most fuel-rich mixtures within and downstream of the duct. Soot formation could be prevented if the richest mixtures can be maintained at equivalence ratios of approximately two or lower in the autoignition zone [1];
- To limit over-mixing at the radial periphery of the spray, enriching the most-fuel-lean mixtures, lowering both hydrocarbon and carbon monoxide emissions. In other words, the duct can help to reduce and narrow the distribution of equivalence ratios reacting at the lift-off length [1];
- The proximity of the duct inlet to the cooler wall of the combustion chamber could tend to draw cooler charge gas from the thermal boundary layer into the duct; furthermore, the duct itself might be cooler than the ambient in-cylinder gases. Both of these phenomena could lead to cooler mixtures within the duct, allowing more mixing to occur during an increased ignition-delay period [1];
- To have leaner mixtures at the duct exit, bringing to longer ignition delays due to chemical-kinetic effects, providing more time for pre-mixing [1].

Hereafter, the DFI technology [2] is depicted in terms of flame structure:

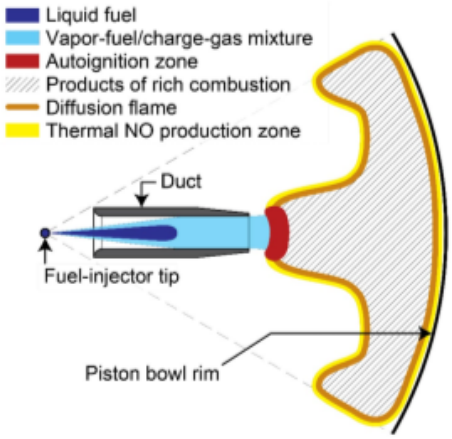

Figure 1: DFI technology and flame structure

2. Experimental Reference

The developed activity has been based with respect to the experimental results achieved by Sandia National Laboratories, which tested the improvements of the DFI technology by introducing fully optical equipment: the constant volume combustion vessel [3]. This gear enables to directly observe and easily reproduce the flame evolution and stabilization under a wide range of thermo-chemical conditions, similar to the one observed in most practical fields wherein combustion plays a main role.

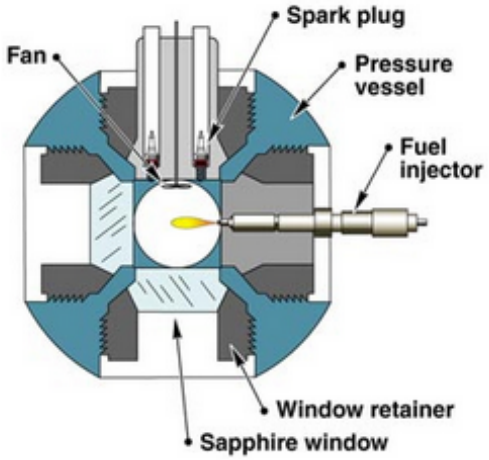

Figure 2: Experimental Sandia CVCV

The duct used, named with an efficient convention, for the experimental campaign is the D2L16G3.9δ: diameter of 2mm, length of 16mm, stand-off distance of 3.9mm, and δ corresponding to geometry with tapering around the outer diameter to 0.5mm wall thickness at the duct exit. The same duct geometry will be also used for basing the numerical investigation.

3. Methodology

The target of this work is to create a numerical model able to reproduce, in the most accurate way, the actual DFI state-of-the-art represented by the results achieved by Sandia National Laboratories during its experimental campaign. To do that, some assumptions have been made relative to all the different aspects involved in a turbulent combustion process, modeling the way the fuel spray may evolve in space and time due to the presence of ambient air.

3.1. Numerical Setup

The approach adopted in order to investigate the DFI technology is numerical, and it has been conducted thanks to the CFD software OpenFOAM. Initially, the computational domain has been created so to be geometrically identical to the experimental one. The creation of the mesh grid is case-dependent since the introduction of the duct profile requires a further constraint to the domain generation: the common choice is the higher mesh grid density in the closeness of the injection axis, so to have an accurate solution of the CFD computation in those regions. Furthermore, an axisymmetric 2D domain has been chosen for the CFD simulations: in this sense, less computational effort is required and the transient evolution of the system is independent of the chosen reference plane.
For what concerns the injection system, the choice has been oriented toward the same gear adopted by Sandia National Laboratories for the investigation of the Spray A case, the $A210370$, with an axial orientation and an operating injection pressure of 150 MPa. The injection duration has been set to 4ms, a sufficient time for a quite-exhaustive evaluation of the combustion process. The kind of considered fuel is the n-dodecane, characterized by a 99% purity level.
The ambient air has been considered a perfect gas with a constant density, equal to 22.8 $\frac{kg}{m^3}$, and it has been assumed to be near-quiescent so that its velocity field is negligible compared to the one of the fuel jet. The turbulent pattern in the combustion vessel has been described by introducing the k-ε model: the choice of this kind of model is due to its simplicity and effectiveness in reproducing a turbulent environment. Con-

sidering the turbulence, all the simulations have been solved thanks to the RANS approach.
For the spray evolution description in space and time, the assumption of a constant spray cone angle has been adopted, with a uniform droplet size distribution at the exit of the injection nozzle. The KHRT model [4], which considers both the Kevin-Helmholtz and Rayleigh-Taylor dynamic instabilities, has been used to describe the fuel jet breakup due to the aerodynamic and viscous influence of the ambient air. To express the heat transfer process between fuel droplets and the ambient air, the Ranz-Marshall model has been considered.
The analysis of soot production related to both FJ and DFI combustion processes has been defined by introducing the Leung-Lindstedt-Jones model [5], which enables the description of the soot formation process, subdivided into three different steps: nucleation, surface growth, and oxidation.

	Model
Breakup	KHRT
Heat Transfer	Ranz-Marshall
Turbulence	$k-\varepsilon$
Soot	Leung-Lindstedt-Jones

Table 1: Models for the analysis of the combustion process

Moreover, two different combustion models have been considered for the modeling of the CFD process, assuming that the flame front can be decomposed according to the flamelet approach: PSR and ADF. The introduction of the flamelet model enables to decouple the effects that chemistry and physics have on the transient evolution of the system toward the equilibrium condition achievement, due to the different time scales associated with them. The two combustion models are then characterized by some differences, according to the influence turbulence has on the sub-grid level chemical structure of the system:

- *PSR*: the impact of turbulence is not considered and thus the system evolution only depends on chemical reactions. Moreover, in each cell of the computational domain, the chemical composition is not affected by any kind of gradient.
- *ADF*: the impact of turbulence is very important, so the system evolution both depends on chemical reactions and mass diffusion, described by the *scalar dissipation rate*, χ. Thus, inside each cell, the chemical composition is characterized by a gradient depending on the turbulence length scale.

For both combustion models, the mixing line assumption has been neglected, whereas fuel evaporation has been considered.

3.2. Model Validation

The main target is to assess whether the numerical model used for the CFD simulations is accurate enough to reproduce and approximate the experimental data, associated with the ECN spray A case: in this sense, the same injector system and thermo-chemical conditions inside the vessel have been modeled. The ambient temperature inside the environment has been conventionally set to 900K and no oxygen has been considered: this means that the attention is focused on the fuel spray evolution inside the vessel, once the thermo-chemical environment has been set. The analysis has been oriented toward the comparison of the mixture fraction field and jet penetration, expressed in terms of liquid and vapor phases. For what concerns the evolution of the fuel spray inside the vessel, it has been evaluated at both 25mm and 45mm from the injection point so to have a better understanding of the impact that environment has on the fuel jet, in terms of both interactions with the surrounding air and subsequent turbulence generation.

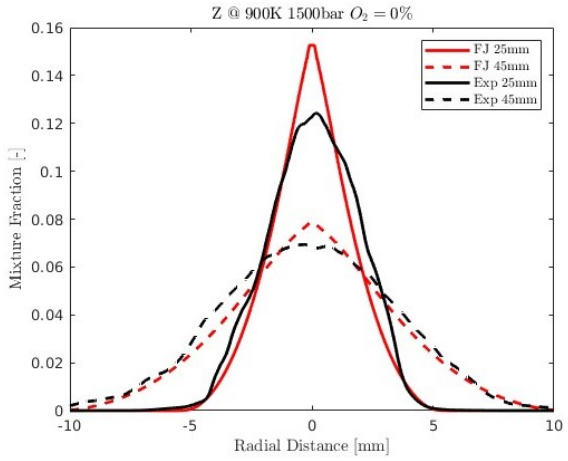

Figure 3: Mixture fraction field comparison between numerical (red) and experimental results (black)

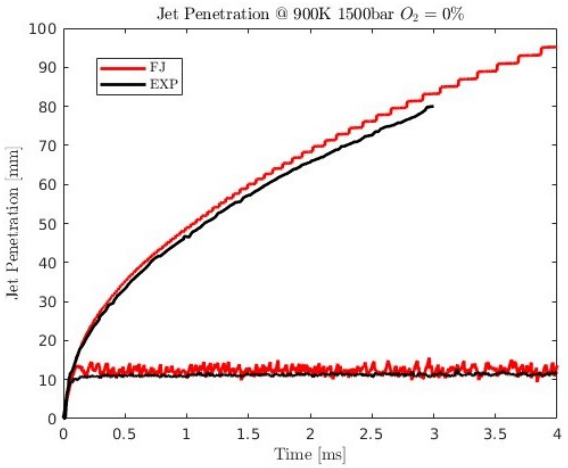

Figure 4: Spray penetration comparison between numerical (red) and experimental results (black)

Although some little discrepancies between numerical and experimental results, which may depend on the kind of approach used for the phenomenon evaluation and thus on the applied tolerances, the global behavior of the numerical model seems to accurately reproduce the experimental spray A case, so the model can be considered as successfully validated.

4. Result and Discussions

The validation of the numerical spray model and the reactive analysis of FJ and DFI cases have permitted to highlight the main differences in terms of flame generation and stabilization inside the vessel. In particular, the following study is oriented to the analysis of the combustion process, under the following boundary conditions:

	value
Oxygen Amount	15%, 21%
T_{amb} **[K]**	850, 900, 950
Combustion Model	PSR, ADF

Table 2: Analyzed operating conditions for the reacting case

By considering these operating conditions and models, the activity target is the evaluation of similarities between numerical results and experimental trends of the main flame features associated with DFI technology, so to assess which combustion model better reproduces the actual state-of-the-art. Two significant quantities for a first step of analysis are the ignition delay time (IDT) and the lift-off length (LOL), where hereafter are presented the values at 21% of O_2 with a sweep of temperature:

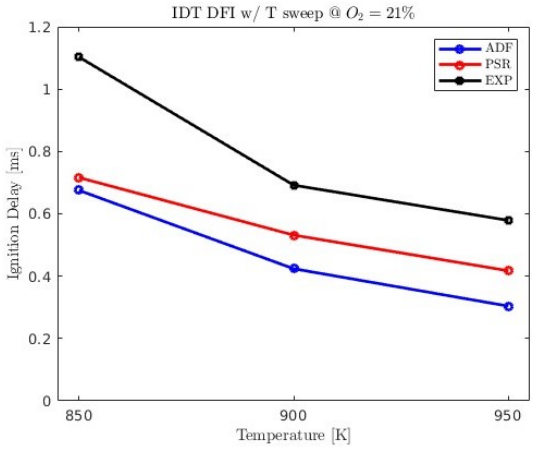

Figure 5: Ignition delay time (IDT) comparison between numerical (PSR and ADF) and experimental results

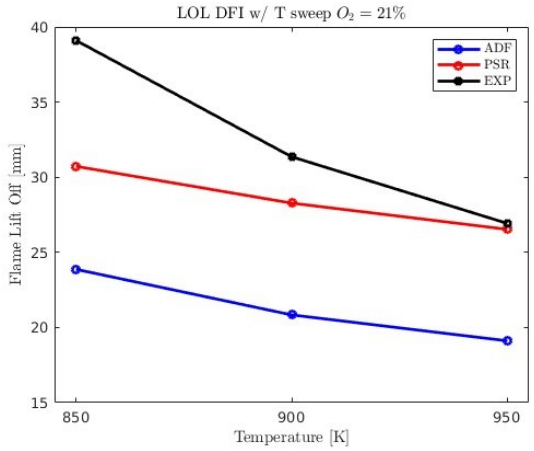

Figure 6: Lift-off length (LOL) comparison between numerical (PSR and ADF) and experimental results

By looking at the previous results, it is possible to appreciate that both the two combustion models underestimate the experimental results associated with flame generation and stabilization in the case of an LTC. Nevertheless, the PSR model is able to better reproduce the actual DFI experimental state-of-the-art: the increase in temperature determines global improvements for the reproduction of the experimental trend. Due to the fact that at both 15% and 21% O_2, the PSR has turned out to be the most accurate in reproducing the DFI combustion experimental results, only this model has been considered to study the soot production.

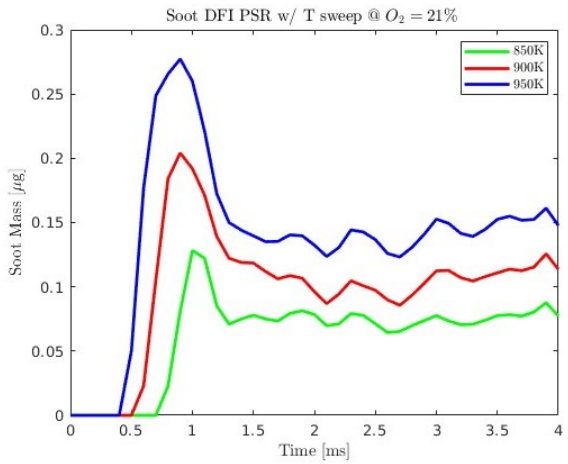

Figure 7: Soot for DFI technology at 21% O_2

Some considerations can be done by looking at the previous results: soot production is affected by the thermo-chemical state of the vessel and, thus, by the ambient temperature and oxygen concentration. Considering the vessel temperature, the higher this one, the lower will be the time window available for the mixing between fuel and air, and thus the volume of partially-oxidized products will be bigger. In particular, for the DFI case, the effect the temperature has on the soot volume production seems to be more influential than the contribution of the ambient O_2 concentration: a temperature increase of 100K corresponds to a maximum soot production raise of 120%. On the other side, the soot production seems to be independent of the ambient O_2 concentration, once the thermal state of the vessel has been set. Nevertheless, the higher oxygen concentration determines, at the same temperature, a higher peak of soot formation: having a larger amount of oxidizer means reducing the time required for the generation of an ignitable air-fuel mixture. The similarity of soot production profiles for the DFI technology at 15% and 21% O_2 is strictly linked to the evolution of the equivalence ratio, Φ field inside the vessel: a brief comparison between the 2 thermo-chemical states is hereafter proposed

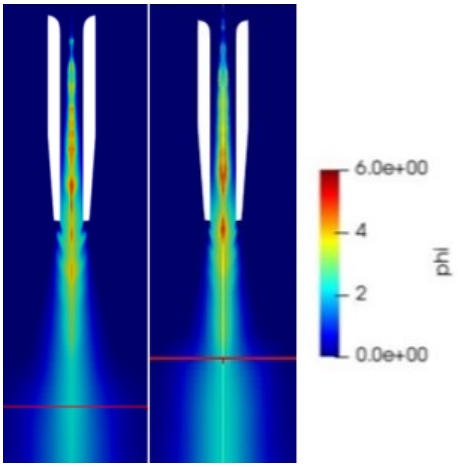

Figure 8: Equivalence ratio field for DFI at 15% and 21% O_2

Moreover, for the sake of simplicity, here it has been reported only the soot comparison between the FJ and DFI at the ambient temperature of 900K: this choice is due to the will of emphasizing the main differences between the two combustion techniques, giving a measure of all the improvements the DFI approach is able to introduce with respect to the conventional way.

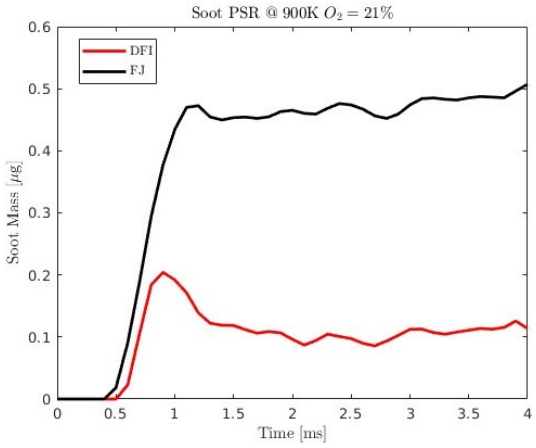

Figure 9: Soot production comparison between FJ and DFI at 21% O_2

5. Conclusions

The activity presented in this thesis has the aim of pointing out the improvements, in terms of soot reduction, that the DFI technology introduces with respect to the conventional process characterized by a free-spray jet. Starting from the experimental state-of-the-art defined by Sandia National Laboratories, a numerical model has been created for reproducing in the most accurate way the results associated with the Spray A case: under no-reacting conditions, it has been demonstrated the similarity between the numerical model with the experimental result. Once the model has been validated, the step forward was the comparison, under reacting conditions, between the numerical results with the experimental ones related to the main traits associated with flame generation and stabilization: the LTC case has been considered, and two different combustion models have been used to assess which of them is the most accurate for reproducing the Sandia National Laboratories results.
The best model has then been employed for the analysis of soot production, and results show some interesting conclusions:

- Once the ambient oxygen concentration has been fixed, the effect ambient temperature has on the soot production is more evident for the DFI technology rather than the conventional free-spray case: by considering the same range of temperatures, an increase of 100K determines an increase in soot production for the DFI 10 times higher than the free-spray;
- The soot production with the DFI is more likely to be associated with the air entrainment upstream of the duct and the turbulent mixing after the duct exit, thus more related to the duct geometry and pressure drop rather than the ambient O_2 concentration;
- The presence of the duct delays the ignition time and allows to further downstream the ignition location than the free-spray one and this leads to a longer lift-off length (LOL). The increase in LOL leads to a higher entrainment rate and better air-fuel mixing. Consequently, this leads to a reduction of soot precursor.

The present study highlights how the adopted numerical model produces results in line with the current state-of-the-art, in addition, the DFI technology introduces huge improvements concerning the soot reduction for each analyzed thermo-chemical condition of the vessel. It is worth underlining how the current model can be considered idoneous for future studies.

References

[1] Charles J Mueller, Christopher W Nilsen, Daniel J Ruth, Ryan K Gehmlich, Lyle M Pickett, and Scott A Skeen. Ducted fuel injection: A new approach for lowering soot emissions from direct-injection engines. *Applied energy*, 204:206–220, 2017.

[2] Christopher W Nilsen, Drummond E Biles, and Charles J Mueller. Using ducted fuel injection to attenuate soot formation in a mixing-controlled compression ignition engine. *SAE International Journal of Engines*, 12(3):309–322, 2019.

[3] ECN. Engine combustion network, 2023.

[4] Jennifer C Beale and Rolf D Reitz. Modeling spray atomization with the kelvin-helmholtz/rayleigh-taylor hybrid model. *Atomization and sprays*, 9(6), 1999.

[5] Kin M Leung, Rune P Lindstedt, and William P Jones. A simplified reaction mechanism for soot formation in non-premixed flames. *Combustion and flame*, 87(3-4):289–305, 1991.