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Development of a multi-component based methodology for the simulation of reacting high injection pressure Diesel sprays

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Abstract

Modern Diesel engines are attractive for fuel economy and performances but they are suffering from increasingly strict emission standards. Therefore the investigation of the injection and combustion processes are mandatory. This paper focuses on the development of a multi-component fuel based methodology for the simulation of non-reacting and reacting high injection pressure Diesel sprays.

In multi-dimensional modeling fuels are represented predominantly by single components, such as n-Dodecane for Diesel, and this is a limitation in their ability to represent real fuels which are blends of hundreds components. This study outlines a method by which the fuel composition is represented by means of a Discrete Multi-Component (DMC) model approach in order to improve the prediction of the vaporization behavior of high injection pressure Diesel sprays.

A testing blend of 6 hydrocarbons is taken into account and a reduced one is developed in order to reduce the computational cost of the CFD simulations while maintaining the advantages due to a multi-component description of the mixture. The CFD methodology is developed within Star-CD commercial code while particular care is also dedicated to the prediction of the atomization and secondary breakup processes. At the nozzle exit the atomized droplets are predicted by a primary breakup approach which is able to take into account the cavitation phenomena and the turbulent effects. The atomization model is based on a simplified approach that is able to evaluate the effects of the nozzle geometry.

The preliminary investigations are performed in a constant volume vessel, validating the numerical parameters against experimental data in order to correctly reproduce spray vaporization behavior. Then, to illustrate the important differences between the vaporization characteristics of a multi-component mixture compared to a mono-component one, the CFD methodology is tested investigating the in-cylinder combustion process of a 4 cylinders, Common Rail Diesel engine of current production.

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1. Introduction

Constant improvements in injection systems, turbocharger design and after treatment systems have allowed the Direct Injection Diesel (DID) engine to become very attractive for automotive applications with low fuel consumption, improved specific power and excellent drivability. On the other hand Diesel engines suffer from stringent new pollutants emissions regulations and in this context design improvements can be assessed using CFD in order to understand and optimize engines design [1, 2].

However, the numerical codes implemented for engine simulation need further development to become fully predictive. This represents a particular challenge because many complex phenomena are involved related to unsteady turbulent flow, liquid spray, combustion and pollutant formation and being coupled in a high temperature and high pressure environment [3] as the engine cylinder is. Understanding and modeling the behavior of the dispersed phase [4] and the combustion mechanisms [5] are essential to improve engine performance.

The aim of this paper is to improve the simulation of reacting high injection pressure DI Diesel sprays, developing a new multi-component Diesel mixture. Furthermore a reduced three-component mixture is presented in order to limit the computational cost while maintaining the advantages given by the multi-component approach. The present simulations allow to assess the ability of the multi-component approach to account for changes of the investigated parameters and therefore to reproduce the experimental trends. In particular the predictivity of the engine performance and the sensitivity of pollutant emissions during different operating conditions are investigated.

The predictive capability of a RANS based CFD methodology is presented comparing results of evaporating sprays against standard lagrangian RANS and LES simulations by means of a numerical fluid dynamic commercial code.

The paper is structured as follows: the multi-component mixtures are first described and then the spray and combustion modeling are presented. The experimental results used to validate the spray modeling are introduced and then a comparison between the different atomization models is carried out. The effects of the multi-component approach are then analyzed in a constant volume vessel. Finally, the combustion process is simulated by means of the ECFM-3Z model, adopting a simplified approach based on a single fuel vapor component and injecting the multi-component fuel in a 4 cylinders Common Rail Diesel engine of current production.

2. Discrete Multi-Component approach

As real Diesel may have up to several hundred fuel components [6] to model the real fuel as a multi-component mixture a simplified approach is required. Two different means of modeling multi-component fuels exist. By the first, the fuel is modeled as discrete fuel species, the characteristics of which are determined from existing chemical libraries. For the second the fuel is treated as a continuous species and the fuel composition is described by a probability distribution function (PDF) based on molecular weight. Boiling point or carbon number [7] and fuel properties are so deduced from this PDF [8]. While commercial fuels can be composed of hundreds of hydrocarbons, most fuels can be accurately modeled with a few components ($\leq$10) and for this reason the discrete multi-component model approach is developed. As far as the composition of the commercial Diesel is not fully known, for this activity the composition of a simplified Diesel is adopted. It is characterized by 6 hydrocarbons whose families are given by Thomas et Al. [9] obtained with the analysis of some samples of commercial Diesel. In particular that analysis identified three main compounds families and the percentage by mass composition as visible in Table 1.

Table 1. Multi-component composition and mass percent

Hydrocarbon class	6 components mixture	%	Reduced multi-component	%
Paraffins	n-Dodecane	25.0	n-Hexadecane	57.0
	n-Hexadecane	19.0		
	n-Octadecane	13.0		
Alkylbenzenes	Toluene	4.0	Ethylbenzene	8.0
	Ethylbenzene	4.0		
Alkyl-napthalenes	1-Methylnapthalene	35.0	1-Methylnapthalene	35.0

In order to reduce computational costs due to the introduction of 6 scalar equations, representative the components mixture, a reduced 3 components Diesel formulation is adopted and reported in Table 1.

The multi-component fuel model considers the mixture as an ideal solution and it is able to mix even up to infinite different fuel components. The model is then completed adopting polynomial or other type of functions able to reproduce the thermo-physical properties as a function of the temperature according to [10].

The bulk properties of the 6 components mixture and of the reduced one are close to those of the commercial Diesel used in the in-cylinder experimental activity.

3. CFD Methodology

The CFD simulations are carried out by the commercial code Star-CD [11]. The turbulence is modeled by means of the RNG k-ε approach, as implemented by Yakhot et Al. [12] and for the dispersed phase, the standard Lagrangian approach is adopted.

Concerning the primary breakup process, a new atomization model [13], developed for GDI spray applications, is investigated. Turbulent effects are then taken into account in the equations describing the wave growth in the liquid fuel; the simplified approach introduced by Huh and Gosman [14] is modified and a contribution of the effects generated by the cavitation is superimposed. The new approach provides a simplified yet generalized estimation of the flow conditions adopting basic and well-known injector characteristics. The primary breakup model predicts an initial droplets distribution at exit of the nozzle holes, while the atomization process is completed by the Kelvin-Helmholtz instabilities as developed in the Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) hybrid model [15]. The KH-RT hybrid model is then used to model the secondary breakup process of the fuel droplets.

The evaporating/condensing droplet mass transfer is expressed as [16] where a mass coefficient is introduced by the formulation of El Wakil [17] and, as far as a multi-component formulation of the fuel is adopted, the surface area of the droplet accounts for the mass fraction of the component *i*.

The combustion process is modeled by the ECFM three zone (ECFM-3Z) combustion model[18]. The ECFM-3Z is based on the Extended Coherent Flame Model (ECFM) which has been developed at IFP for spark ignition engine applications. The correlation determined by Ryan & Callahan [19] was chosen to compute the auto-ignition delay. EFCM-3Z includes a description of the auto-ignition process by integrating in time the auto-ignition delay based on the equivalence ratio and temperature. In the ECFM-3Z the diffusion flame is simply represented by a Magnussen type model. As the oxidation process continues, the formation of pollutants (soot and NO_x) is taken into account. The soot formation is described using a homogeneous mechanism presented in [20] while the NO formation is described by the extended Zeldovitch model.

4. Results and discussion: constant volume vessel, no reacting diesel spray

In order to validate the new atomization model previously described in [13] for high pressure Diesel injection, CFD simulations of the spray from the Engine Combustion Network (ECN) are performed. The table 2 summarizes the experimental data [21].

Table 2. Sandia experimental configuration

Fuel	n-Dodecane (n-C12H26)	Injection duration	1.5 ms
Nozzle Outlet Diameter	90 µm	Injected fuel mass	3.5 mg
Discharge Coefficient	0.86	Ambient gas temperature	900 K
Fuel injection pressure	150 MPa	Ambient gas pressure	6.0 MPa
Fuel injection temperature	363 K	Ambient gas density	22.8 kg/m^3

4.1. Lagrangian setup: atomization and break-up model comparisons

A uniform computational grid made up of hexahedral cells of 1 mm^3 of dimension [22] representing the experimental quiescent chamber, is used to validate the CFD methodology. In the present work the effects of the grid resolution on the n-Dodecane spray evolution are also investigated even considering a grid made up of hexahedral cells of 0.5 mm^3 of dimension.

The numerical setup based on the new atomization model coupled with KH-RT hybrid break-up model is validated against experimental data and compared to the simulations which adopt well-known numerical models such as the BLOB model and the Huh-Gosman model with the Reitz-Diwakar approach for the secondary breakup of the droplets. As far as KH-RT hybrid break-up model is concerning, for this activity the B1 tuning constant is set to 40.0 and the C_3 tuning constant to 0.1, referring to [11]. Aiming to improve the prediction of the vapor phase and consequently the air-fuel mixing capability of the numerical setup, the RANS based simulations are compared against the LES-Smagorinsky model.

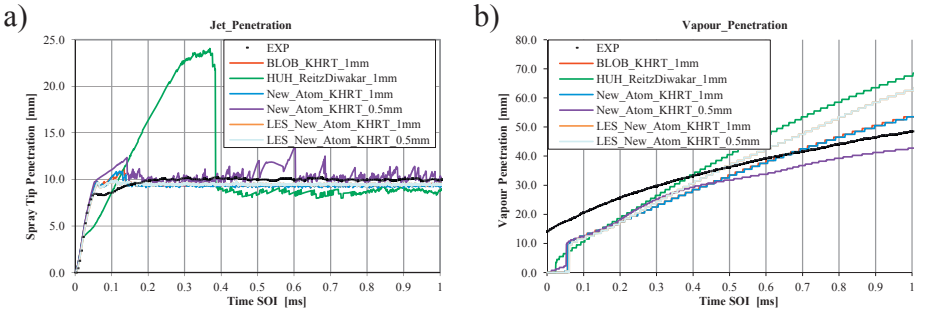

Fig.1(a) Jet Penetration, Fig.1(b) Vapor Penetration

The figures 1(a) and 1(b) show the jet and vapor phase penetration of the simulated sprays compared to experimental data. The figure 1(a) shows that all the atomization models are able to predict the correct jet penetration, while the Huh-Gosman atomization model combined with the Reitz-Diwakar break-up model shows an overestimation of the jet penetration until 0.4 ms. Concerning the grid sensitivity, it can be seen that the differences between the two computational grids (1 mm against 0.5 mm) are not so remarkable. Indeed, since the chamber conditions are evaporating, the jet penetration is mainly governed by the evaporation phenomena and, as reported in figure 1(b), it is expected the fuel vapor penetration is mainly dependent by the computational grid resolution. Thus the prediction of vapor phase is strongly affected by the break-up models, the grids resolution and the turbulence models, as visible in the figure 1(b). It is necessary to remark the numerical setup based on the KH-RT break-up models show a good numerical and experimental comparison. On the contrary the approach of the Reitz-Diwakar model is not able to correctly reproduce the diffusion of the fuel vapor.

As far as the turbulence models are concerned, the simulations carried out using 1 mm grid, overestimate the vapor penetration after 0.4 ms after SOI, while the 0.5 mm grid simulations show underestimated results comparing to the experiments. The LES-Smagorinsky case with 0.5 mmm strongly reduces the gap with experiments in the second part of the injection process.

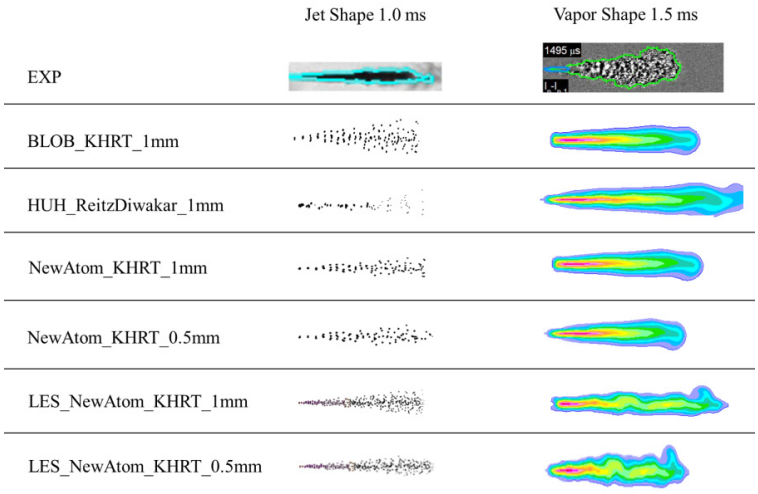

Fig.2 Jet and vapor shape comparison

In order to point out the differences between the BLOB and Huh cases and the new atomization model, the jet shape is investigated in the figure 2. The computational parcel distribution, calculated by the new atomization model, shows a good agreement with the experimental image of the liquid phase, while the BLOB case and the Huh case are not able to reproduce the experimental cone angle. The remarkable numerical and experimental comparison of the new atomization model is due to the improvement in the prediction of the atomization of the droplets far from the liquid column.

As the dimension of the computational cell is reduced and the simulation of the gas-jet interaction is enhanced, the CFD simulations improve the simulation of the liquid spray diffusion as visible for the computational grid of 0.5 mm. Both the RANS and LES approaches to the turbulence show an acceptable spray cone angle. It is remarkable the increasing number of droplets obtained in LES simulations is only due to the reduced time-step required for LES simulations, since a fixed number of numerical parcels per time step is adopted.

The figure 2 shows also the numerical and experimental vapor phase shape of the spray. The vapor fuel diffusion is not correctly simulated by the RANS cases even if a uniformity distribution of the vapor on the edge of the spray is not expected, due to the nature of the turbulence approach. Contrariwise, an improvement in the CFD simulation can be found adopting the LES-Smagorinsky turbulence model, since the vapor shape is predicted more accurately.

The results show that the new atomization model improves the high injection pressure Diesel spray jet simulation, meanwhile the LES approach points out great potential in vapor shape prediction.

4.2. Diesel fuel modeling: comparison between mono and multi-component mixtures

In view to deeply investigate different vaporization behavior of the mixtures, in this section a comparison between the mono- and the multi-component mixture is reported. The comparing simulations are performed injecting the fuel in the constant volume vessel, as far as the previously validated CFD setup is adopted: the new atomization model, the KH-RT break-up model and the RANS k-ε RNG turbulence approach are chosen.

The figure 3(a) shows the total evaporated mass over the total injected liquid mass. The evaporation rate is different between mono- and multi-component mixtures, while the three-component and the six-component mixtures have similar behaviors; it is evident that the mono-component fuel evaporates first if compared to the multi-component mixtures. As described in [13], referring to gasoline fuel mixture, it can be assumed that the multi-component mixture is more consistent with the real fuel mixture as the simplified three-component mixture shows a good compromise between accuracy (figure 3(a)) and reduced computational cost (figures 3(b)).

The figure 3(b) reports the computational costs of the adopted CFD fuel setup, compared to the standard pure Diesel fuel. As expected, the increased number of the scalar equations, representing the vapor phase of the fuel components, increases the computational time of the solver. The computational cost highly increases when considering one scalar for each component.

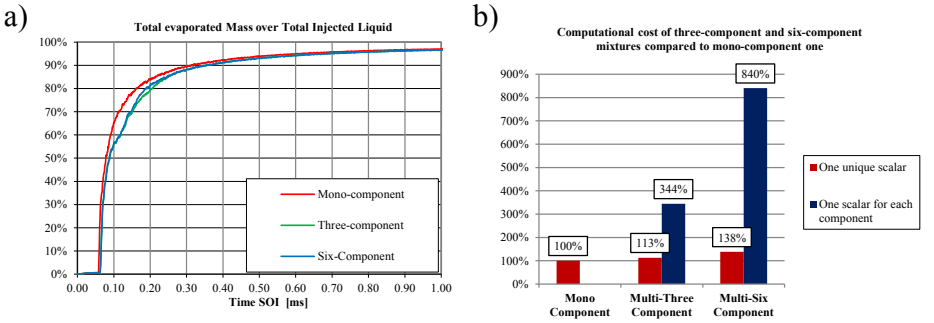

Fig.3(a) Total evaporated mass over total injected liquid, Fig.3(b) Computational cost of three- and six–component mixtures compared to mono-component one

Since in this preliminary investigation of the multi-component approach for the simulation of the fuel mixture, the combustion process and the simulations of the complete engine cycle are performed by means of the ECFM-3Z combustion model, a simplified use of the vapor scalars equations is required. Due to the fact the equations of ECFM-3Z model takes into account just one reacting vapor scalar, in this activity, the vapor phases of the two investigated multi-component mixtures are let to evaporate in a single averaged vapor scalar. Even though some vapor scalars properties are missing and the potentialities of the multi-component mixtures is reduced, the computational load of the simplified approach is reduced as visible in the graph of the figure 3(b) which shows the three-component and the six-component mixtures have a computational cost comparable than mono-component one.

As a final remark, the figures 4(a) and 4(b) show the percentage of the rate of evaporation of the single components for the three-component and six-component mixtures. As the fuel droplet is totally evaporated the percentage of vapor correctly reproduce the initial liquid fuel composition.

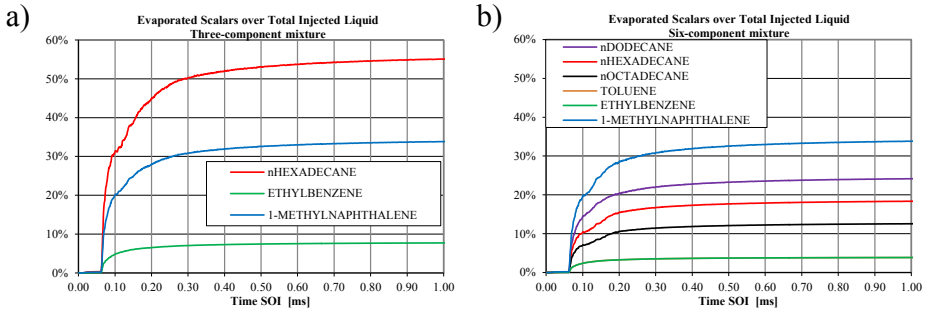

Fig.4(a) Evaporated scalars over total injected liquid – Three-component mixture, Fig.4(b) Evaporated scalars over total injected liquid – Six-component mixture

5. Results and discussion: in-cylinder simulations

In order to point out the improvement in the simulation of injection and combustion processes using a multi-component approach, in-cylinder simulations of a 4 cylinders Common Rail Diesel engine of current production are

carried out. The engine cycle is simulated by means of the Star-CD commercial code, the new atomization model coupled with the KH-RT break-up model is chosen to model the injection process and the RANS RNG k-ε model is adopted as turbulence approach.
The intake phase process, the in-cylinder flow field and the combustion process are simulated adopting a fully 3D grid, as depicted in figure 5. Concerning the computational grid resolution, a mean cell width of 0.5 mm is used. The engine specifications are described in table 3 and the two investigated engine operating conditions are reported in table 4.

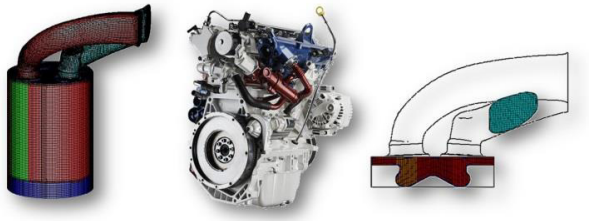

Fig.5 Common Rail Diesel Engine and Fully 3D computational mesh used

Table 3. Engine specifications

Bore [mm]	69.6
Stroke [mm]	82.0
Compression ratio	17.6:1
Connecting rod length [mm]	131.3
Valves/Cylinder	4
Number of holes	6
Injector hole diameter [μm]	121

Table 4. Operating Conditions

Case	A	B
Engine speed [rpm]	4000	2000
Load	Full	Partial
Injection pressure [MPa]	160	80
Pre-Injection	No	Yes
Start of Injection(SOI) [°CA BTDC]	21.5°	8.0°
Injection time [ms]	1.56	1.52
EGR [%]	0	10

The initial conditions and the boundary conditions are derived from 1D CFD calculations previously performed by the commercial code GT-Power and from experimental data. Three different fuel mixtures are used: mono-component mixture, three- and six-component mixture . Droplet-wall interactions and liquid film transport including evaporation and boiling are also taken into account.

Due to the complexity of the in-cylinder turbulence phenomena and the dependency from the initial condition [23] of such transient phenomena, the LES modeling of the turbulence generation during the in-cylinder cycle is not taken into account for the in-cylinder simulations.

5.1. Case A: 4000 rpm full load

Figure 6(a) compares the simulated mean in-cylinder pressures to the experimental curve, during the combustion process for the case A, while figure 6(b) focuses on the comparison of the in-cylinder pressure peak. It can be seen the six-component approach slightly improves the simulation results compared to the three-component and the

mono-component case. The burnt mass fraction is reported in the Figure 7(a), which shows that only the six-component mixture behaves differently compared to the mono-component one, while the three-component mixture has a similar trend to the mono-component one.

The multi-component fuel approach reveals a particular improvement as far as the pollutant emissions are compared to experimental data at the exhaust valve opening (EVO), as visible in the figure 7(b). The three-component mixture improves the pollutants prediction if compared to the mono-component simulation and the six-component mixture further improves the prediction if compared to three-component calculation. Concerning the prediction of CO emissions, an improvement of the CFD methodology is mandatory as far a deeper investigation of the predictive capability of the soot model.

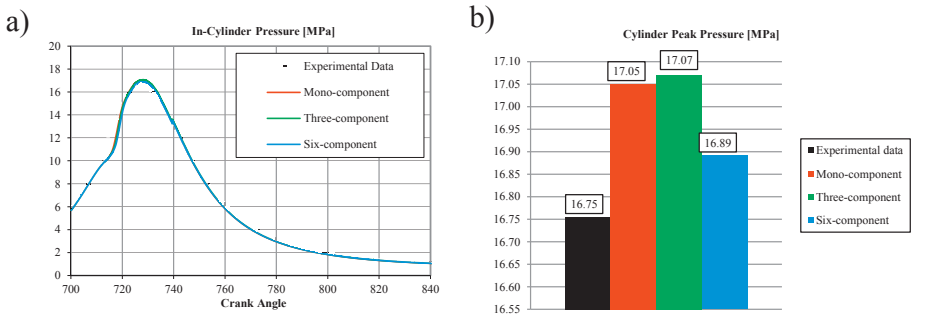

Fig.6(a) Comparison between computed and experimental in-cylinder pressure at 4000 rpm full load, Fig.6(b) Comparison between computed and experimental in-cylinder peak pressure at 4000 rpm full load

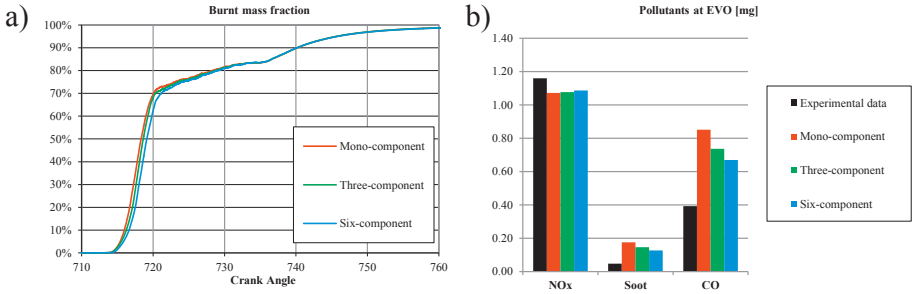

Fig.7(a) Burnt mass fraction at 4000 rpm full load, Fig.7(b) Pollutants at EVO at 4000 rpm full load: comparison between computed and measured data

5.2. Case B: 2000 rpm partial load

As far as the partial load engine condition is investigated (case B), a multi-injection strategy is adopted. The figures 8(a) and 8(b) show a similar trend to the case A. The adoption of the six-component approach strongly reduces the gap between numerical and experimental in-cylinder pressure and it is remarkable that the different rate of evaporations of the multicomponent mixtures influences the combustion process at such operating engine condition.

Observing the burnt mass fraction (figure(9)(a)) and pollutants quantities at the exhaust valve opening (EVO) (figure(9)(b)) advantages can be found in the implementation of the multi-component mixtures. The mono-component mixture burns first if compared to the multi-component ones. The figure 9(b) shows, indeed, that the multi-component mixtures improve the pollutants prediction. This trend is the same seen for the 4000 rpm full load case.

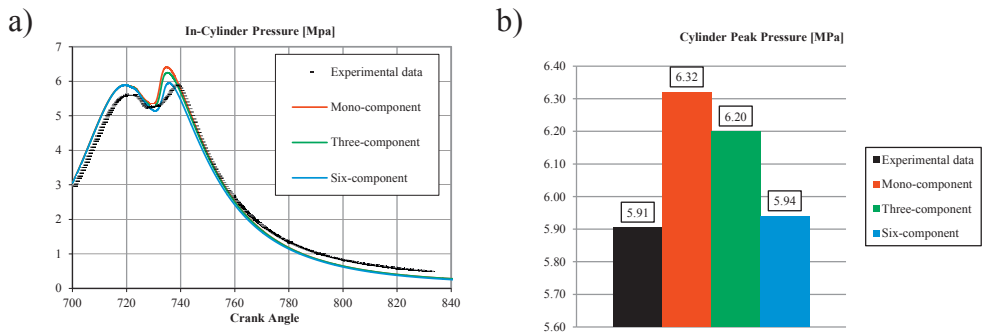

Fig.8(a) Comparison between computed and experimental in-cylinder pressure at 2000 rpm partial load, Fig.8(b) Comparison between computed and experimental in-cylinder peak pressure at 2000 rpm partial load

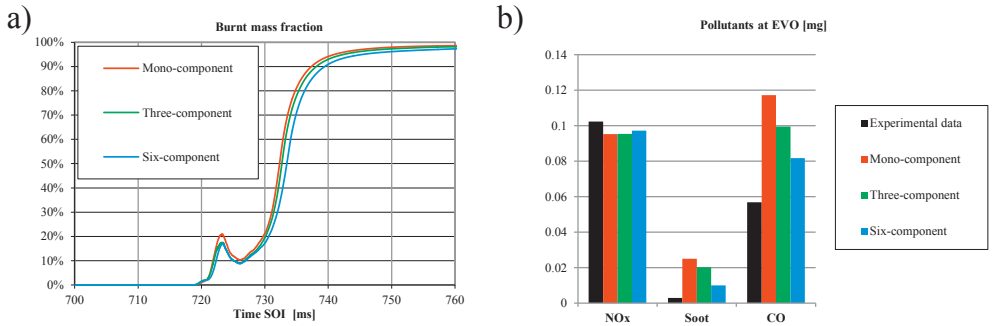

Fig.9(a) Burnt mass fraction at 2000 rpm partial load, Fig.9(b) Pollutants at EVO at 2000 rpm partial load: comparison between computed and measured data

6. Conclusions

This preliminary activity aims to improve the predictive capability of the CFD simulations preserving to be feasible for the industrial applications. Different multi-component Diesel fuel mixtures have been investigated by means of a discrete approach.

A new atomization model, formally developed for GDI injector, has been used to simulate high pressure injection Diesel spray. Since the jet and the vapor phase of the computed Diesel spray correctly approximate the experimental measurements and images, the lagrangian setup showed acceptable results. It has also been reported that using a LES turbulence model, the vapor phase prediction could be improved.

The investigation of the fuel compositions showed that the multi-component mixtures behave differently from the mono-component Diesel as regard the total evaporated mass. The three- and the six-component mixture behave similarly, even though the three-component has a reduced computational cost. In view to investigate the effects of the discrete multicomponent approach, in-cylinder simulations have been carried out and two different engine operating conditions have been simulated. The two analysis proved the multi-component approach slightly improve the prediction of the engine performances (i.e. the in-cylinder pressure) while it influences the prediction of pollutant emissions; best results have been reported for the six-component mixture. Despite the promising results, additional developments are still required so that numerical simulations become fully predictive. Further investigations will focus more specifically to use more than one unique reacting scalar, in order to take the most advantage in the use of multi-components mixtures and it is to pointed out that the dependency of the auto-ignition process from the vapor mixture must be enhanced.

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