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Effects of fuel composition on charge preparation, combustion and knock tendency in a high performance GDI engine. Part II: LES analysis

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Abstract

As discussed in the Part I of this paper, a numerical activity is carried out in order to analyse the effects of fuel composition modelling in a turbocharged GDI engine for sport car applications. While Part I analyses the "ensemble averaged" macroscopic effects on spray evolution, mixture stratification, combustion and knock tendency, in Part II of this paper cycle-to-cycle variations are analysed and discussed using a multi-cycle LES numerical framework, again comparing results from a more traditional single-component fuel surrogate model to those of a multi-component one. A purposely developed numerical approach is applied to properly account for the effects of the Discrete-Continuous-Multi-Component fuel formulation on the charge preparation: just before the spark timing, each vaporized fuel fraction is lumped back into a single-component surrogate fuel to allow the combustion model (ECFM-3Z, in its LES formulation) to take place. At the beginning of a new injection process, the numerical framework for the injected spray is switched back to Multi-Component, thus allowing each fuel fraction to independently spread, vaporize and diffuse in the combustion chamber according to the cycle-specific characteristics. A detailed comparison between the two fuel formulations is carried out on both average and rms values of the most influencing fields just before the spark discharge.

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Keywords: LES; DCMC; mixing; combustion

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1. Introduction

The ongoing request for fuel efficiency increase and pollutant reduction is pushing towards more and more detailed CFD simulations in the field of ICEs. One area of poor detail is fuel modeling. This is due on one hand to a general shortage of detailed data in literature regarding fuel properties, due to their chemical varied nature, and on the other hand to the complexity of advanced numerical models and their CPU cost when coupled with a real engine simulation. For these reasons the consolidated approach in fuel modeling in ICE applications relies on a single species (i.e. Single Component, SC), whose physical properties are usually fitted as a function of temperature. Among all the physical properties involved, the saturation pressure (or vapor pressure) strongly affects the rate of transition from liquid to vapor and should be as corresponding as possible to that of the actual fuel. What makes this aspect so critical in DI engines is that the phasing of fuel vapor formation affects charge stratification. A reliable fuel distribution at the end of the compression stroke is a fundamental condition for an accurate combustion simulation.

The difficulty in simulating real fuels lies in their complex blend of hundreds of hydrocarbons of different nature. They are usually grouped in classes following their molecular structure: olefins, aromatics, paraffins, oxygenated additives etc. This composition variety is often represented as a quasi-continuum spectrum of molecular weights present in the fuel, implying the coexistence of chemical compounds whose evaporation behavior is very different.

The lightest components have a fast evaporation tendency, and their partial pressure is relatively high even at low to moderate temperatures. On the contrary, the heaviest components have a low vapor pressure over a wide range of temperatures. This makes them the substances needing the longest time for a complete evaporation.

The overall evaporation dynamics of such a real fuel is expected to immediately involve the most volatile components, due to their higher vapor pressure. As these start the transition to the vapor phase, the average composition of the liquid moves towards higher molecular weights, as the heaviest components have not experienced enough time to evaporate. The evaporation of such heavy components is expected to be the most critical for many ICE applications in terms of limited evaporation and mixing time for charge stratification formation before combustion ignition.

The picture is even more complex considering cycle-to-cycle variability (CCV) of in-cylinder turbulent flows. CCV is an undesired phenomenon affecting the cyclic behavior of a real engine, whose characterization is well known in the field of ICE research [1,2]. This influences cylinder filling, fuel mixing, flame kernel formation and flame front development, all of these exhibiting fluctuations between consecutive engine cycles for the same operating conditions.

This Part II of the study is intended to continue the analysis undertaken in Part I, focusing on the investigation of the fluctuations of mixture stratification. This is carried out through a comparison between the consolidated SC approach and a more refined DCMC methodology. In the next section an overview of the analyzed engine is given, then the numerical methodology is described both in terms of fuel modeling and LES combustion simulation. Finally the results from the two simulation frameworks (SC and DCMC) are analyzed and compared in terms of charge stratification and combustion behavior.

Nomenclature

AFR	Air-to-Fuel Ratio
CCV	Cycle-to-Cycle Variability
CoV	Coefficient of Variation
DCMC	Discrete-Continuous-Multi-Component
DI	Direct Injection
ER	Energy Resolution
FSD	Flame Surface Density
LSR	Length Scale Resolution
SC	Single Component

2. The engine

The investigated engine is a 8 cylinder V-shaped highly turbocharged direct injection spark ignition (DISI) engine, whose characteristics are reported in the Table 1.

Table 1. Engine parameters

Displacement	≈ 3800 cm3
Bore/Stroke Ratio	> 1
Max Power	> 500 kW @ 7000rpm

The studied operating point is the same investigated in Part I, i.e. it is the 7000rpm WOT full load/peak power one, which is indicated as knock-limited one by the engine manufacturer.

3. Methodology

The numerical framework for the Large-Eddy Simulation (LES) is here reported, with particular focus on the fuel modeling technique. All the CFD analyses are carried out by Star-CD v4.20, licensed by CD-adapco.

The difference between SC and DCMC method is in the formulation of the fuel vapor pressure. In the SC method, the fuel composition is synthesized as C_7H_{13} and its vapor pressure law is given as a fitted function of temperature. This is suggested by the fuel manufacturer and implemented in the CFD code through user coding. Moving to the DCMC implementation, the adopted surrogate model is the 7-components blend suggested for a commercial gasoline by Batteh et al. [3] and reported in Table 2. For each of these constituents a dedicated vapor pressure curve is user provided as a function of temperature.

Table 2. DCMC fuel components as in [3].

Component	Mass fraction
Butane	4%
Pentane	16%
Hexane	2.5%
Toluene	25.5%
Octane	32%
Benzene	18%
Tridecane	2%

As the current study aims at evaluating the improvements brought in by a multi-component simulation, the only difference between the two simulation realms is the specification of the saturation pressure. The other liquid fuel properties used in the simulations (liquid density, latent heat of vaporization, isobaric specific heat and surface tension) are measured by the fuel supplier as a function of temperature and they are defined as invariant for SC and DCMC simulations.

Fuel spray atomization is simulated by means of user coding [4], while Reitz's model is adopted for secondary breakup and Bai-Gosman's model is chosen for droplet-wall interaction. This latter aspect is critical for such a wall-guided GDI engine. However due to the very high piston temperature at full load/WOT condition, no liquid film model is used in the simulations.

Wall temperatures are imposed as a fixed value for each component, although the fluid-solid interaction is currently under evaluation through a CHT analysis [5]. Boundary conditions at inlet and outlet sections are given in terms of time-varying pressure and temperature, whose values are extracted from a tuned 1-D model used by the engine manufacturer.

Combustion is simulated by means of the ECFM-LES combustion model [6], using the Flame Surface Density (FSD) concept which has been widely used in previous works regarding CCV [7,8] in DI engines. The same approach for combustion adopted in Part I is here applied and now briefly resumed. The simulations with the multi-component DCMC approach needs a dedicated treatment prior the combustion modeling. This consists in grouping

(i.e. 'lumping') the vapors of the 7 components forming the fuel surrogate model into a single fuel, whose properties are the same as the fuel used in the SC simulations. The reasons for this are twofold. The first is strictly numerical, as the adopted implementation of ECFM-LES combustion model requires a single fuel species. The second motivation is more general and lies in a non-consistency which is found in literature whether multi-component formulations for the evaporation of real fuels are valid models also in term of combustion properties (e.g. lower heating value, laminar burning velocity etc.) or not. What it is usually found is that the fuel surrogate model is targeted to match the evaporation rate of the reference fuel, while no validation is given in terms of its combustion behavior. This lumping approach offers the advantage to perform a combustion simulation on a mixture stratification given by a spray modeled with a DCMC approach, and as shown in Part I the impact on spark ignition and knock tendency in the end-gas can be remarkable.

Ignition is modeled by means of the AKTIMeuler ignition model, which is based on a FSD deposition at spark time.

The computational mesh used in the simulations is often a concern in LES simulations, being the main responsible for non-affordable CPU costs in an industrial context. The grid used in this study consists of approximately 1.5 million cells at BDC. The full geometry must be considered in the LES framework, since no hypothesis on symmetric flows can be exploited as in Part I of this paper using a RANS approach. The adopted mesh was extensively validated in terms of grid quality requirements for LES analysis [9], both considering the Energy Resolution (ER) criterion and the Length Scale Resolution (LSR) one. Both indicators proved this computational grid to be sufficiently accurate for the LES analyses. Finally the model used for subgrid scale viscosity is the Smagorinsky one, in its static formulation. The numeric schemes adopted are 2^{nd} order for momentum, temperature and turbulence, while 1^{st} order was used for time discretization.

A total of five full-cycles are simulated for each of the two approaches, and the presented results constitute a preliminary comparison between the two methods for spray evaporation. Each simulation requires approximately 96 hours on a 48-core Linux workstation. Despite the reduced number of realizations to draw converged statistics, to the author's opinion the available results allow a first investigation of the differences between the two models.

4. Results

4.1 Spray Evaporation Discussion

The focus of this section is on fuel evaporation and stability in consecutive cycles. The global vapor fuel which is formed during the engine cycle is reported in Fig. 1a-b for the SC and the DCMC methods. Obviously, in the DCMC framework a total of 7 different vapors is formed during spray evaporation, one for each fuel component. In order to carry out a coherent comparison with the SC approach, an "equivalent fuel vapor" concept is exploited, being this the sum of the 7 vapor concentrations.

The ensemble average curves give a first characterization of the overall evaporation rate, with the DCMC formulation undergoing a slower evaporation process than the SC method in average terms, as reported in Fig. 1-a. This is in agreement with the outcomes from Part I of the study. A visual confirmation of this is in Fig. 2, where the same cycle is compared for SC and DCMC approach at BDC. The DCMC cycle exhibits a still large population of liquid droplets compared to the SC one, alongside with overall leaner mixture formation.

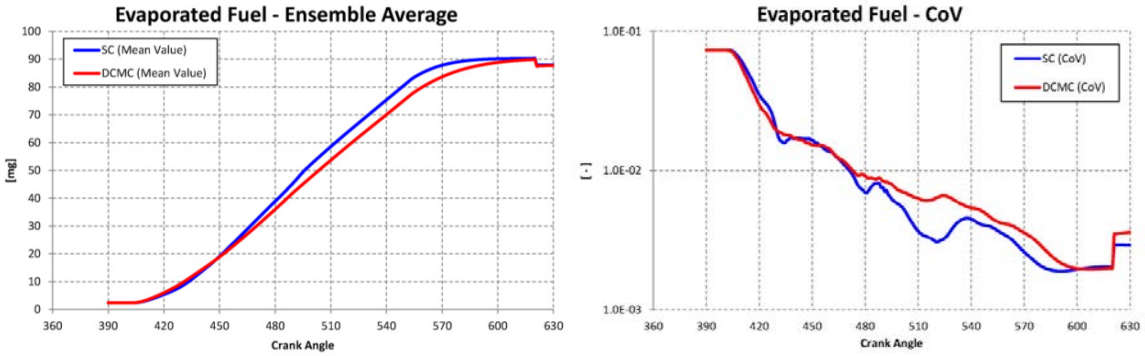

Fig. 1. (a), left: ensemble average curves of fuel for SC and DCMC methods; (b), right: CoV of fuel vapor formation.

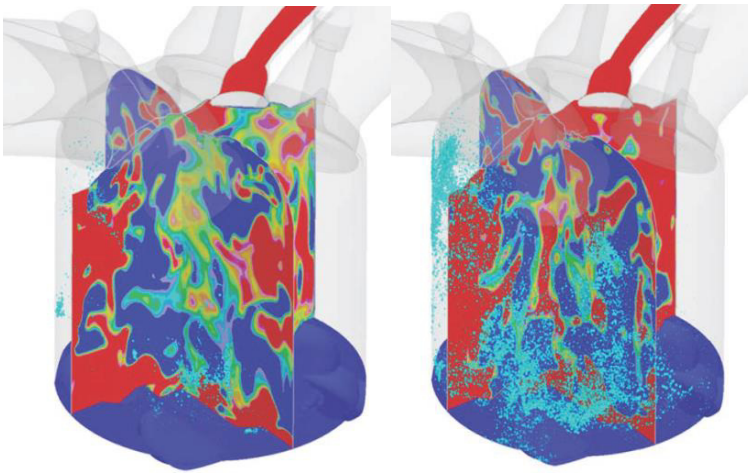

Fig. 2. Air index (scalar field) and liquid droplets at BDC. (a), left: SC; (b), right: DCMC.

The variability in mixture formation between different cycles is represented by the Coefficient of Variation (hereafter CoV) of the fuel vapor, expressed for a given time as the ratio between the rms of the vapor mass in all the simulated cycles (i.e. their CCV) and the ensemble average. The normalization with the mean value is carried out to separate the amplitude of the measured fluctuation from the global faster/slower evaporation rate for SC/DCMC. This variability is given by the interaction of the GDI spray with cycle-specific turbulent flow realizations.

In the first part of the injection phase (say up to 480CA), both methods exhibit the same CoV (i.e. comparable CCV), while in the second portion (say after 480CA) the CoV of the DCMC method is higher than that of the SC one. Finally the CoV indicators re-align in the final portion, as the mixing process reduces the concentration peaks after end of injection. The DCMC method predicts an overall higher variability in the amount of vapor fuel between consecutive cycles compared to the SC one, and this is due to the evaporation of the heavier compounds as it is now demonstrated. In fact, the DCMC method allows a further level of investigation, i.e. the analysis of each component constituting the 'equivalent fuel'. This investigation confirms that the lightest components (e.g. C_4H_{10} and C_5H_{12}) undergo a general faster phase transition to vapor than the high-boiling ones (e.g. C_9H_{12} and $C_{13}H_{28}$). The mean evaporation rate of each component is reported in Fig. 3-a. In order to carry out a coherent comparison between all the components, whose presence in the fuel blend can be very different (see Table 2), each of them is normalized by its percentage weight in the DCMC fuel model adopted.

The longer is the time needed for the liquid phase to evaporate (i.e. high-boiling components) the shorter is the time for mixing once the vapor phase is formed. This is of crucial importance for the heaviest substances, behaving

as the main responsible for CCV of charge stratification at the end of the compression stroke. Again, this is expressed by the CoV indicator, now separately applied for each vapor component.

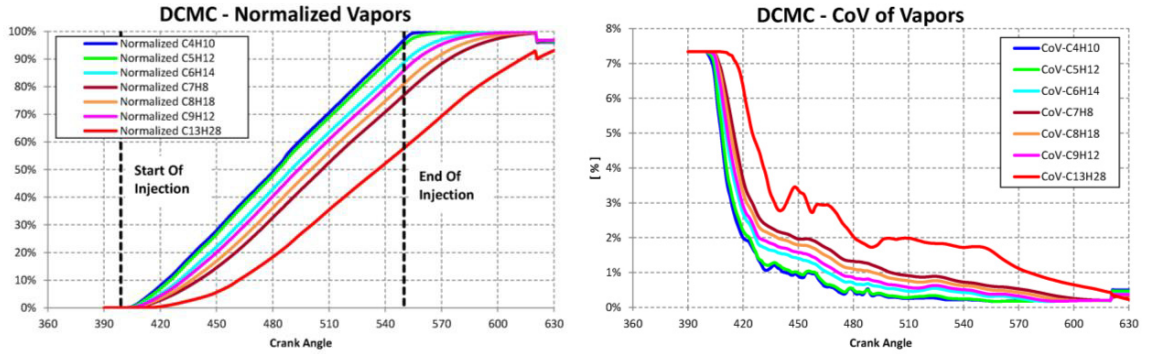

Fig. 3. DCMC component-specific evaporation history. (a), left: normalized evaporation progress; (b), right: CoV.

The CoV for all the 7 components is reported in Fig. 3-b throughout the injection life cycle and the evaporation phase. It is evident how the lightest hydrocarbons are less affected by evaporation fluctuations than the heaviest ones. This is verified for the lightest/heaviest components, while intermediate ones present a bias from this trend. The higher charge homogeneity for the lightest substances is due to their higher vapor pressure for a given temperature. In particular, the evaporation rate is driven by the difference between the saturation pressure of the fuel and its instantaneous partial pressure, which is null at the beginning of the injection process for all of the components. As already discussed, the faster evaporation for the lightest components allows them a relatively prolonged mixing time, leading to a good charge homogeneity at the end of the compression stroke.

The temperature distribution in the liquid phase is measured at three CA during the injection process: 450CA, 540CA and 630CA. For each observation time a statistical distribution of the liquid temperature is carried out for every cycle, and the results are reported in Fig. 4-5-6.

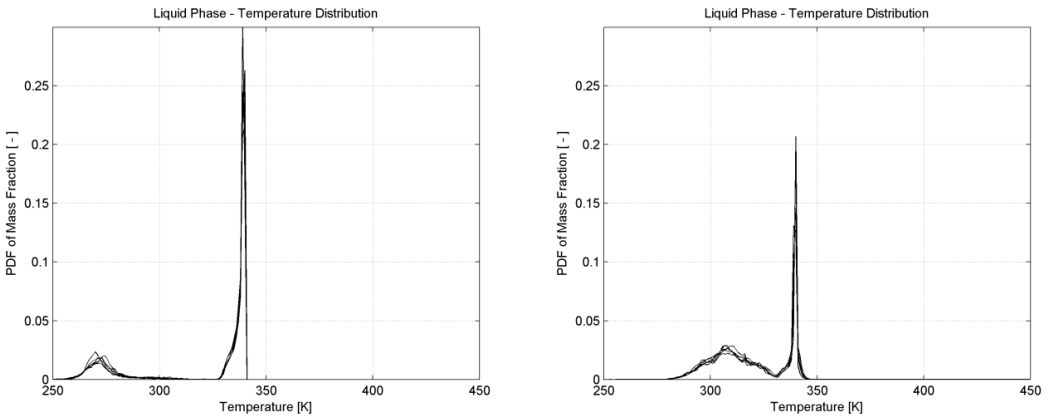

Fig. 4. Temperature distribution in the liquid phase at 450CA. (a), left: SC method; (b), right: DCMC method.

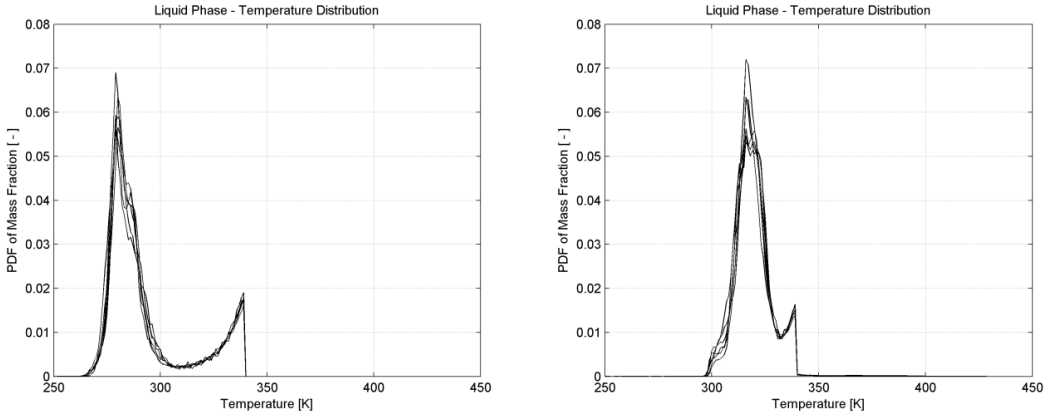

Fig. 5. Temperature distribution in the liquid phase at BDC. (a), left: SC method; (b), right: DCMC method.

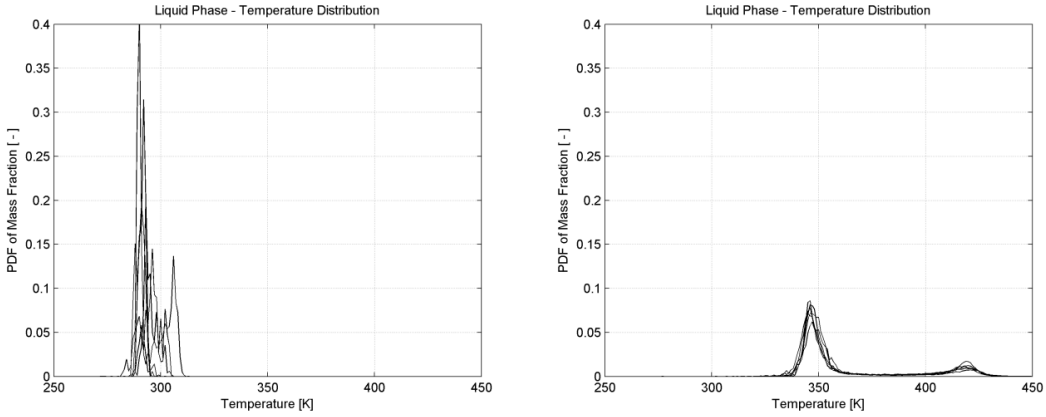

Fig. 6. Temperature distribution in the liquid phase 630CA. (a), left: SC method; (b), right: DCMC method.

The initial temperature of the injected liquid fuel is 340K for both methods. This value is derived from a detailed injector characterization provided by the engine manufacturer and it is an input in the simulations. It is visible how the temperature of the droplet population progressively lowers from the initial value, as a consequence of the heat subtracted by the droplets phase transition. At the beginning of evaporation, the temperature distribution shows a quasi-bimodal condition, with most of the liquid phase close to the initial temperature (spray core) with some reduced probability at lower temperatures (evaporation cooling at the spray plume). Later in the process, the proximity to the initial temperature decreases in probability while distributed thermal density increases, as more liquid mass is composed by dispersed droplets thus increasing the liquid surface for heat exchange processes. Again this is in agreement with the outcomes from Part I in ensemble average terms, while the LES approach depicts differences in the liquid thermal status between consecutive engine cycles.

4.2 Combustion Discussion

The combustion results for the SC and DCMC approaches are presented in this section. The conditions at spark plug proximity are measured at spark time for velocity magnitude and Air Index (Fig. 7). The latter is defined as the actual Air-to-Fuel Ratio (AFR) divided by the AFR at stoichiometry (AFR_{st}). As visible, large variations in both parameters are experienced from cycle to cycle with both SC and DCMC models.

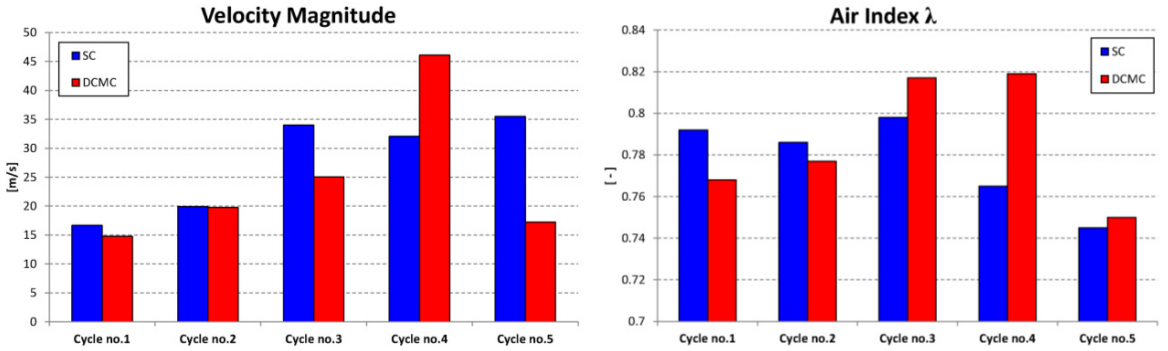

Fig. 7. Conditions at spark for SC and DCMC. (a), left: velocity magnitude; (b): air index.

Table 3. Conditions at spark proximity.

Numeric Approach	CoV of Velocity Magnitude	CoV of Air Index
SC	31.5%	2.8%
DCMC	51.3%	3.9%

While the average values are not significantly varied between the SC and DCMC approach, notable differences are observed between consecutive cycles for both velocity and mixture quality at spark. The fluctuations of these parameters are reported in terms of their CoV in Table 3. The velocity fluctuation at the spark considerably increases adopting the DCMC method, and also the mixture strength variation presents a higher variability. The complex interplay between these factors promotes relevant differences in kernel formation and combustion development.

The combustion results for SC and DCMC cycles are reported in Fig. 8. The combustion CCV is resumed by the peak pressure value history with the two formulations, whose mean and CoV values are reported in Table 4.

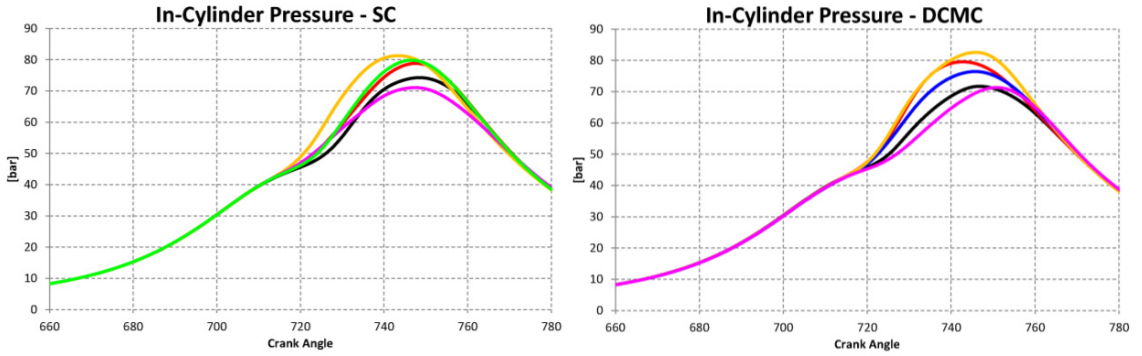

Fig. 8. In-cylinder pressure for SC (left) and DCMC (right) approach.

Table 4. Peak pressure statistics.

Numeric Approach	Average Maximum Pressure [bar]	CoV of Maximum Pressure
SC	77.07	4.94%
DCMC	76.34	5.73%

The average peak pressure is not varying using the two approaches, as a consequence of the same average conditions at spark. However the CoV indicator highlights a relatively high percentage increase in peak pressure

fluctuation with the DCMC approach. This is an effect of the lower charge homogeneity, causing burning rate variations throughout the whole flame propagation process.

5. Conclusions

Two methodologies for fuel evaporation in a highly turbocharged GDI engine are compared, a traditional Single Component (SC) one and a more complex Discrete-Continuous-Multi-Component (DCMC). The study presented in this paper is initiated in Part I, where the two approaches are compared in ensemble average terms thanks to a RANS numerical investigation. In the present paper, the continuation of the analysis is presented for the same engine and operating condition with the focus on the cycle-to-cycle variability of mixture formation and its effects on the predicted combustion stability. To this aim the use of LES technique is necessary and a total of five consecutive full cycles is calculated at the current stage. The ensemble average of LES mixing and combustion results confirm the outcomes from Part I, with a slower evaporation rate found for DCMC method. The value added from LES analysis is the fuel evaporation CCV and its impact on combustion stability given by the longer/shorter exposition of each fuel component to the in-cylinder turbulent flow field. The results show that the heaviest components are those responsible for the largest cycle-to-cycle stratification due to their reduced time for mixing, while the lightest boiling components counterbalance the turbulent fluctuations with a longer mixing time. The SC approach does not allow to perform such an analysis, given the intrinsic mean fuel formulation undertaken. The DCMC method allows to overcome this limitation and the impact on combustion stability is resumed by larger peak pressure fluctuations. The prediction of combustion CCV is thus increased using the DCMC method.

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