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

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Abstract

The paper analyses the effects of fuel composition modelling in a turbocharged GDI engine for sport car applications. Particularly, a traditional single-component gasoline-surrogate fuel is compared to a seven-component fuel model available in the open literature. The multi-component fuel is represented using the Discrete-Continuous-Multi-Component modelling approach, and it is specifically designed in order to match the volatility of an actual RON95 European gasoline. The comparison is carried out following a detailed calibration with available experimental measurements for a full load maximum power engine speed operation of the engine, and differences are analyzed and critically discussed for each of the spray evolution, mixture stratification and combustion.

In the present paper (Part I), a RANS approach is used to preliminarily investigate the behaviour of the fuel model on the average engine cycle. In the subsequent Part II of the same paper, the numerical framework is evolved into a more refined LES approach, in order to take into account cycle-to-cycle variations in mixture formation and knock tendency.

Keywords: RANS, DCMC, mixing, combustion, knock

1. Introduction

Fuel-air mixture preparation, combustion and exhaust gas after-treatment are the noticeable processes in internal combustion engines which control the engine power, efficiency and tailpipe emissions. Due to a cause-and-effect relationship, mixture preparation contains some key pre-processes which relevantly affect the combustion phenomenon, especially in modern direct injected engines. Three main factors are responsible for the mixture preparation features: injected fuel spray characteristics, in-cylinder flow motion and fuel physical properties.

The injection system governs spray phasing, orientation, atomization, droplet breakup and the possible formation of liquid film on the components facing the combustion chamber.

Flow motion is responsible for the deviation of the injected liquid as well as for the subsequent mixing of the evaporated fuel with the inducted air.

Fuel composition affects the evaporation rate and the stratification of different hydrocarbons in the combustion chamber.

A real fuel is a complex blend of hundreds of hydrocarbons of different nature, which are usually grouped in

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classes following their molecular structure: olefins, aromatics, paraffins, oxygenated additives etc. A coexistence of chemical compounds whose evaporation behaviour is largely different is therefore unavoidable. 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 vapour pressure over a wide range of temperatures, which makes them the slowest portion to reach complete evaporation. The evaporation of such heavy components is expected to be the most critical for many ICE applications because of the reduced mixing time before ignition and the increased risk of deposit formation on the relatively cool combustion chamber walls [1]. Since mutual interactions between each single fuel component affect the liquid/gas equilibrium at the fuel droplet surface, the evaporation rate of each component differs from its "single component" behaviour.

The details of multi-component fuel evaporation are still not well understood. Due to the complexity of the involved phenomena, the detailed experimental characterization of fuel evaporation and mixture preparation is far from being feasible in the R&D industrial practice, and it is not trivial even in highly specialized research laboratories. CFD simulations become therefore a valuable (if not mandatory) tool to rationalize and understand the interaction between fuel evaporation, mixing and combustion development. The established approach in fuel modelling in ICE applications still 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, the saturation pressure (or vapour pressure) strongly affects the rate of phase transition from liquid to vapour; it should therefore match as accurately as possible that of the real fuel. This aspect is extremely critical in DI engines, since the fuel vapour formation phasing affects the charge stratification, where a reliable and consistent fuel distribution at the end of the compression stroke is a key condition for an accurate combustion simulation. More detailed CFD approaches in the field of fuel modelling are therefore under development, involving more than one species, mostly developed to better match the distillation curve of the actual fuel.

The task is not trivial, mainly due to the highly variable compositions of the actual fuels and to the lack of detailed data in literature on fuel distillation curves and fuel-component properties. Furthermore, the number of components must be carefully chosen since it affects not only the accuracy of the results but also the complexity and CPU cost of the simulations.

The aim of the work is to investigate the influence of fuel composition on its evaporation under actual engine operations. A single component "equivalent fuel" case is compared to a multi component one within two different simulation frameworks: in the present Part I, the comparison is carried out within the "ensemble average" concept typical of the RANS approach to turbulence modelling, while in the Part II the approach is refined using Large-Eddy Simulation to evaluate the effect of fuel composition on cycle-to-cycle variability.

As it will be demonstrated, fuel formulation strongly influences both air/fuel ratio and local charge temperature distributions, which in turn are fundamental parameters in the evaluation of the combustion process development and the engine knock tendency [2].

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 below.

Table 1. Engine parameters

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

The investigated operating point is the 7000 rpm WOT one, which is indicated as a knock-limited one by the engine manufacturer. With particular focus on mixture preparation and combustion evolution, the investigated operation is of great interest since the engine is fed with a very rich mixture, and the high revving speed strongly reduces the time available for evaporation and mixing.

3. Methodology

In the engine, fuel-rich mixtures are adopted at full-load operations to avoid knock inception and to limit the turbine inlet temperature, this resulting in high levels of brake specific fuel consumption. Since the engine is

operated at the edge of knock, as documented in previous publications [3-5], it provides a useful benchmark not only to assess the influence of fuel composition on mixing and combustion, but also to improve the knock prediction methodology developed by the research group [6,7].

3.1 Multicomponent fuel formulation

The multicomponent approach adopted in the paper is based on the concept of Discrete-Continuous-Multi-Component fuel (hereafter DCMC), in which the population of actual fuel components is lumped into seven main "families", each representing a relevant branch of hydrocarbons. Each family, listed in Table 2 below, contributes with its own mass fraction:

Table 2. DCMC fuel components

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

According to the DCMC concept, each constituent *m* of the fluid mixture, whose local concentration is expressed as a mass fraction , is assumed to be governed by a species conservation equation of the form:

$$\frac{\partial}{\partial t}(\rho Y_m) + \frac{\partial}{\partial y_j}(\rho u_j Y_m + F_{m,j}) = s_m \tag{1}$$

Where $F_{m,j}$ is the diffusional flux component, s_m is the rate of mass production or consumption and Y_m is the local component concentration expressed as a mass fraction. The evaporation of each component depends on the other components because its vapour pressure is a function of the concentration of these component in the mixture.

In order to compute the partial pressure of each component the Raolt's law is applied in the form:

$$p_{vi,s} = X_{i,l} p^0{}_{vi,s} \tag{2}$$

Where $X_{i,l}$ is the component's mole fraction in the liquid and $p^0{}_{vi,s}$ the saturation pressure of the pure substance that constitutes component *i* at the droplet's surface.

The evaporation rate of each component in therefore obtained by:

$$\frac{dm_{di}}{dt} = -\varepsilon_i \frac{W_i}{\sum_{j=1}^n \varepsilon_j W_j} A K_g p_t \ln \frac{(\varepsilon_i p_t - p_{vi,\infty})}{(\varepsilon_i p_t - X_{i,l} p^0{}_{vi,s})} \tag{3}$$

And ε_i is given by:

$$\frac{\varepsilon_i - X_{i,\infty}}{\varepsilon_i - X_{i,s}} = \frac{1 - \sum_{j=1}^N X_{j,\infty}}{1 - \sum_{j=1}^N X_{j,s}} \tag{4}$$

The droplet is considered boiling when the following condition is satisfied:

$$\sum X_{i,l} p^0{}_{vi,s} \geq p_t \tag{5}$$

The choice of the fuel components and of their concentrations is derived from literature [8] and it proves to properly fit the evaporation rate of the actual fuel. For each fuel component, saturation pressure is computed using a sixth order polynomial function of temperature, limited on top by the critical temperature:

$$Ps = \sum_{i=1}^{7} C_i * T^{i-1} \qquad (6)$$

The resulting saturation pressure curves are reported in Fig. 1 below, where the black curve represents the saturation pressure of the single component fuel. The remaining properties (density, specific heat, viscosity, etc.) are derived from the actual ("lumped") fuel and evenly applied to all the components. To increase the accuracy of the simulations, each property is defined as a function of temperature by fitting experimental data provided by the fuel manufacturer.

The DCMC approach is used in the CFD simulations until the start of combustion (SOC), due to both limitations in the combustion model and to the lack of consistency of the adopted fuel formulation (which is valid for the specific purpose of volatility) with the actual fuel chemistry. Right before the spark advance, all the components are lumped in a single one (C_7H_{13}), whose physical and chemical behaviour well represents the actual fuel. The lumping procedure is also adopted to allow the CFD simulations to consistently adopt the tabulated approach for knock prediction which is briefly described below, which is based on the physics and chemistry of a "single component" fuel surrogate accurately matching the autoignition property of a RON95 European gasoline.

3.2 Spray and combustion models

All the CFD analyses are developed in the framework of Star-CD 4.20, licensed by CD-adapco. The simulation of the liquid spray is carried out using a Eulerian-Lagrangian approach. The 7-plume fuel spray is modelled by means of a purposely calibrated user coded routine for primary breakup [9], the Reitz model for secondary break-up and the Bai-Gosman approach for droplet-wall interaction. The actual injected mass-flow profile and the injected droplet properties are specified through user coding. Due to the lack of consistent data for each single fuel component, and considering the full-load engine operation, where the formation of liquid film on the very hot piston surface is unlikely, liquid film formation is not accounted for.

The combustion model adopted for the analyses is the ECFM-3Z, whose well-known suitability for premixed as well as diffusive and autoigniting combustion regimes is a fundamental requirement for the present study. Despite the recent introduction of multi-component combustion models, the adopted version of the ECFM-3Z relies on a single burning fuel, and it is based on a transport equation for flame surface density which takes into account the wrinkling of the flame front surface by turbulent eddies and a conditioning averaging technique which allows precise reconstruction of local properties in fresh and burned gases.

For the diffusive combustion, a description of the mixing state is added, where the "3Z" acronym stands for three different mixing zones: a pure fuel zone, a pure air plus possible residual gases zone and a mixed zone in which the ECFM combustion model is eventually applied.
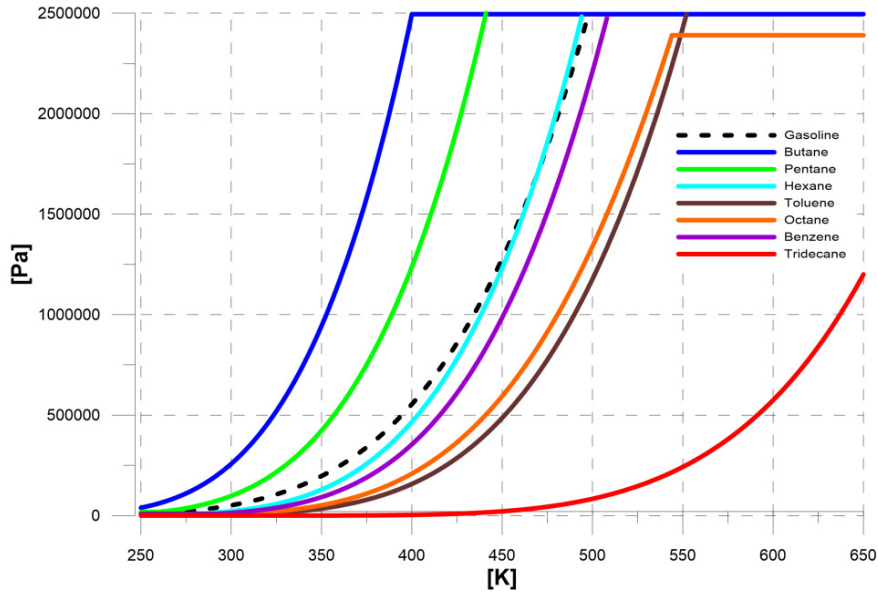
Fig. 1. Saturation pressure of all the components.

Knock is taken into account thanks to a hybrid user-coded/standard formulation, described in details in [6]. It is based on a look-up table for auto-ignition based on the assumption of a single-stage behaviour, in view of the almost null probability of cool flame phenomena or significant low-temperature reactions for the chosen in-cylinder conditions. The look-up table is accessed to reconstruct cell-wise chemical information through local thermo-physical cell state and interpolation.

The selected chemical mechanism for this work is a semi-detailed one based on a Toluene-n-Heptane-Ethanol-Isoctane (THEO) fuel [10], together with a proprietary blend that was provided by the fuel supplier specifically to match the autoignition quality of a commercial European RON95 gasoline. The fuel to be burned is treated in the CFD code as a single-component C_7H_{13} fuel with temperature-dependent properties, being it reasonably representative of a European commercial gasoline.

Once a local autoignition delay is interpolated, the focus shifts to its integration in time to predict knock. The knock model used in the current work is based on the mass fraction of an intermediate fictitious species for autoignition called Y_{IG}, as defined by Lafossas et al. [11]:

$$\frac{dY_{IG}}{dt} = Y_{TF} \cdot \frac{\sqrt{\tau^2 + 4(1-\tau)^{Y_{IG}}/Y_{TF}}}{\tau} \tag{7}$$

A numerical criterion is then adopted to discern the occurrence of knock, based upon the equality between the mass fraction of Y_{IG} and the mass fraction of fuel tracer Y_{TF}, this latter being defined as the "non-reacting" fuel. As the knock model is based on two transported scalars (Y_{IG} and Y_{TF}), it is then straightforward to define a third scalar variable, here called Knock Tolerance (*KT*), as the difference between the two species (2):

$$KT(\vec{x}, t) = Y_{TF}(\vec{x}, t) - Y_{IG}(\vec{x}, t) \tag{8}$$

4. Results

4.1 Experimental validation and droplet analysis

The preliminary validation of the model is based on the average in cylinder pressure trace, reported in Fig. 2 below. As visible, both single- and multi-component fuel simulations accurately match the experiments, thanks to a

careful calibration of the combustion model parameters. The multi-component case required a slight retuning in view of the different equivalence ratio (hereafter ER) distribution, which strongly influences the early combustion stages.
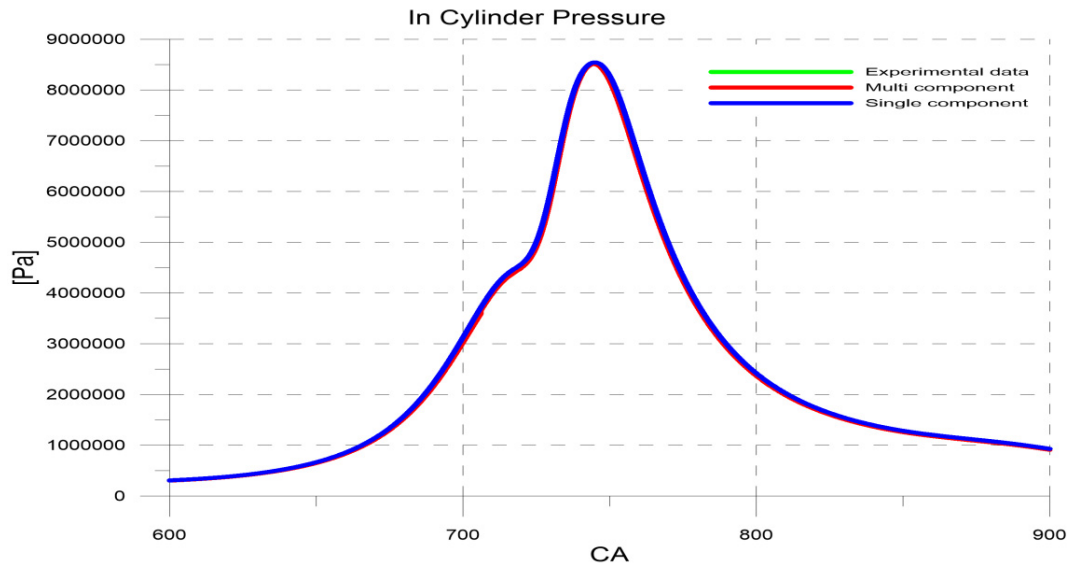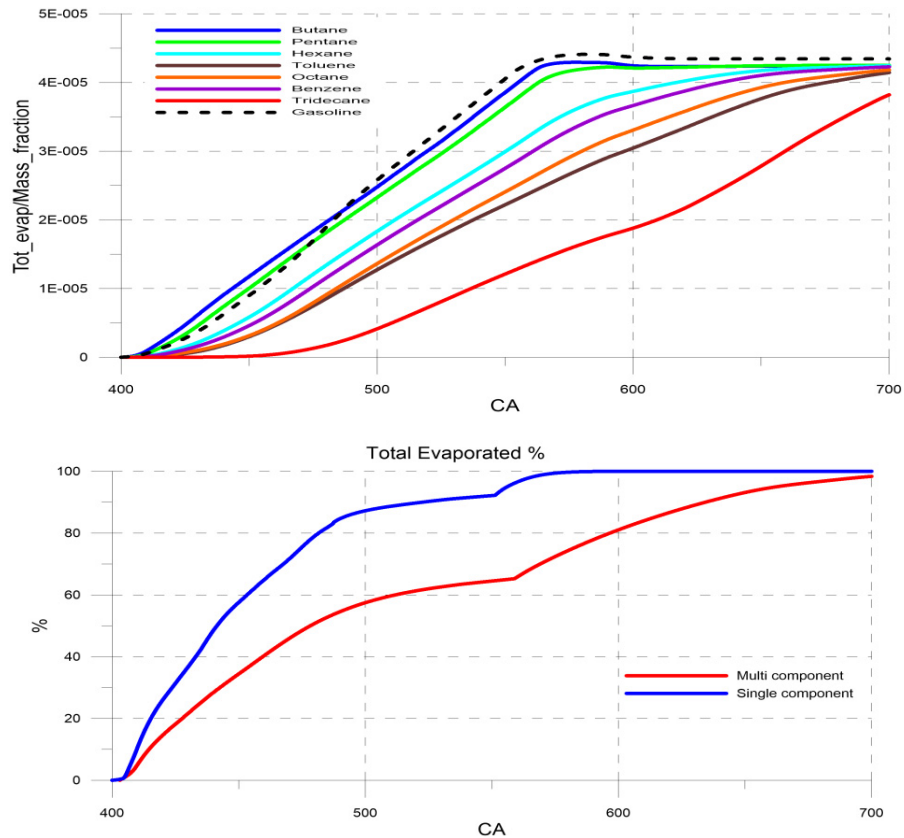

Fig. 2. In-cylinder pressure trace.

Fig. 3. Comparison between the evaporation rate of the single-component and the lumped DCMC evaporation.

Comparing the fuel vapour percentages of the single- and the multi-component fuel simulations it is possible to notice how the DCMC formulation relevantly slows down the evaporation rate throughout the vast majority of the injection and mixing processes. Despite this clearly visible trend, a reverse behaviour can be seen in the very early stage, thanks to the initially faster evaporation of the most volatile compounds. The above considerations are confirmed by the evolution of the liquid phase within the combustion chamber, which is reported in Fig. 4. As visible, in fact, the multi-component case is characterized by a prolonged increase in the amount of liquid phase within the combustion chamber, which reaches its peak value just after BDC. On the contrary, the single component fuel shows an early decrease of the liquid phase, which starts immediately after the end of the injection process.

The cooling of the droplet in the multicomponent case is higher than the other one at the beginning of the injection due to the faster evaporation of the low vapor pressure elements (e.g. butane and pentane).
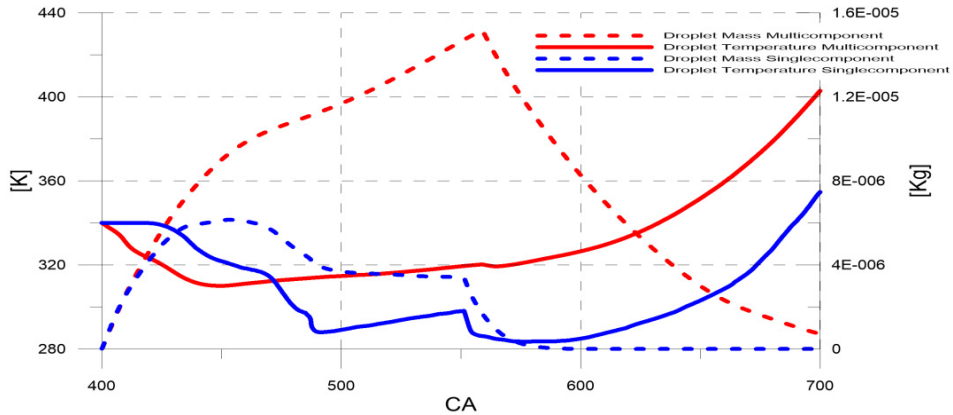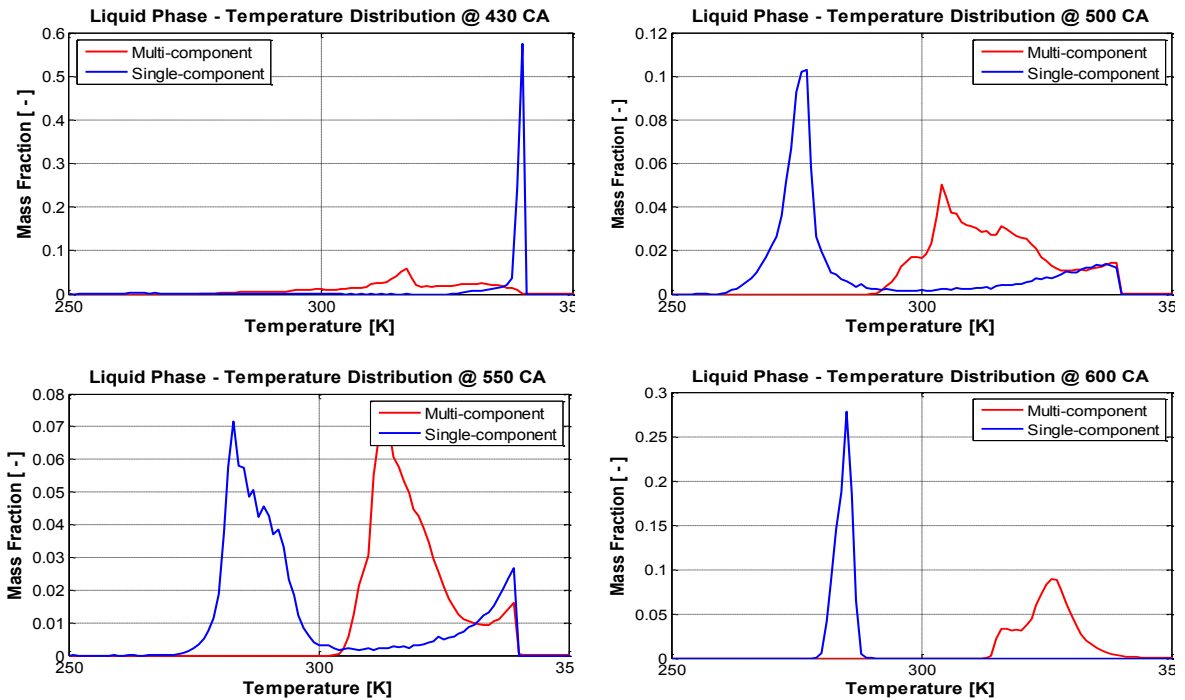

Fig. 4. Mean droplet mass and temperature.

Fig. 5. Statistic temperature distribution of the droplet at 4 different CA.

The droplet temperature trend highlighted in Fig. 4 is confirmed in Fig. 5. Except for the early stage of injection (up to 430°CA) the majority of the droplet population is characterized by higher temperatures in the multicomponent case than in the single component one. This trend is particularly emphasised at 600°CA, in which the two curves are completely separated.

4.2 ER distribution

As introduced before, two of the most influencing parameters in knock inception are mixture quality and gas temperature. The different droplet behaviour seen before promotes different fuel concentrations and different temperature distributions at SOC.

In particular, higher stratification is visible for the multicomponent case: mass distributions of different ER ranges are computed through cells clustering; results are presented in Fig. 7 for three different positions, 540°CA (BDC), 630°CA (mid-compression) and 708°CA (SOC). Due to the slower evaporation, the multi-component case shows a higher population of ultra-lean cells just after the completion of the injection process (540°CA), but the situation is completely reverted towards the end of the compression stroke, since the retarded vapour formation limits proper mixing with the surrounding air.

Furthermore the slower evaporation of the droplets prolongs the charge cooling in the combustion chamber. This is visible for example at the exhaust valve, see Fig. 8 below, which is often a weak point for knock inception in GDI turbocharged engines.
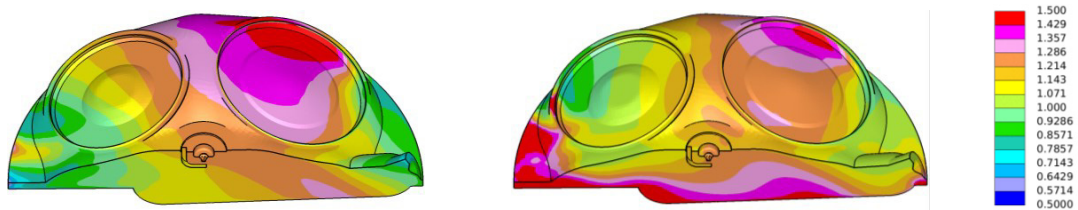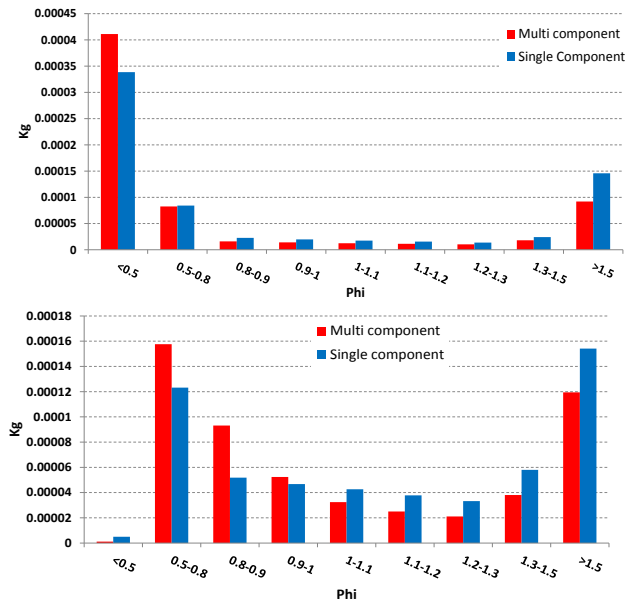

Fig. 6: fuel distribution at SOC (708°CA), Single-Component (left) vs. Multi-Component (right).
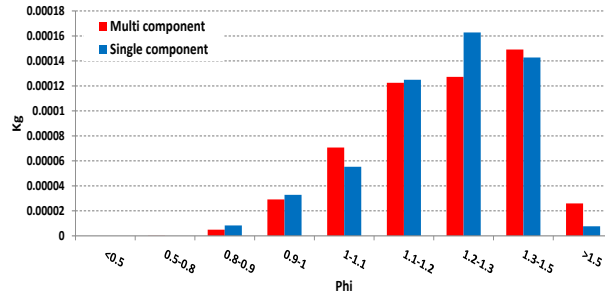
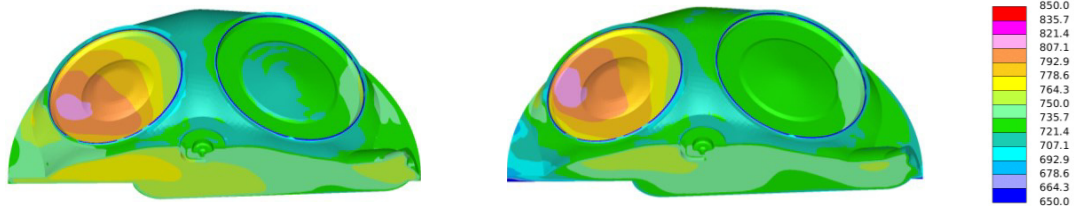Fig. 7: ER distribution @ 540°CA, 630°CA and 708°CA.

Fig. 8: temperature field at SOC (708°CA), Single-Component (left) vs. Multi-Component (right).
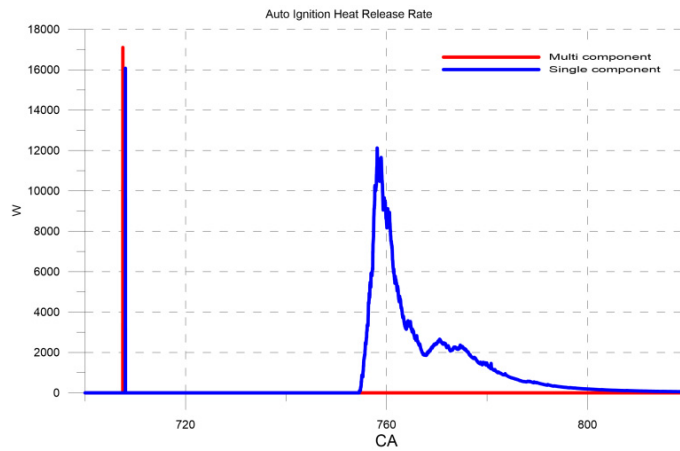
4.3 Knock analysis

Fig. 9. Auto ignition heat release rate.

The heat release rate due to auto ignition in the single component case has the same order of magnitude as the one promoted by the spark, as visible in Fig. 9 above. Since the investigated engine operation is experimentally identified as "close to knock", this result could be accepted even in a "ensemble average" RANS framework The critical zone is located close to the exhaust valve due to the high wall temperatures and favourable equivalence ratios, see Fig. 10.
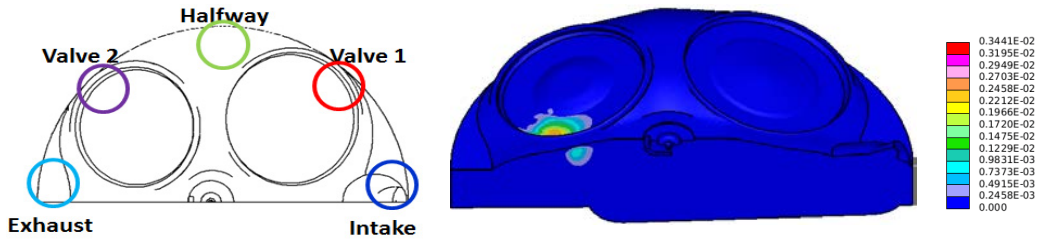
Fig. 10. Sensor position and autoignition heat released [J] at 760 CA.

Still, it is interesting to notice that the residual auto-ignition heat release trace disappears when moving from a single- to a multi-component fuel definition: considering the knock-favourable exhaust side sensor, in fact, autoignition delays increase moving from the single- to the multi-component thanks to slightly richer mixture compositions and slightly lower temperatures, as reported in Fig. 11. Such increase is enough for the flame to reach the critical spot before the autoignition onset, as visible in Fig. 12.

The multi-component approach appears then to be more consistent with the experimental evidence of a "non-knocking" average cycle.
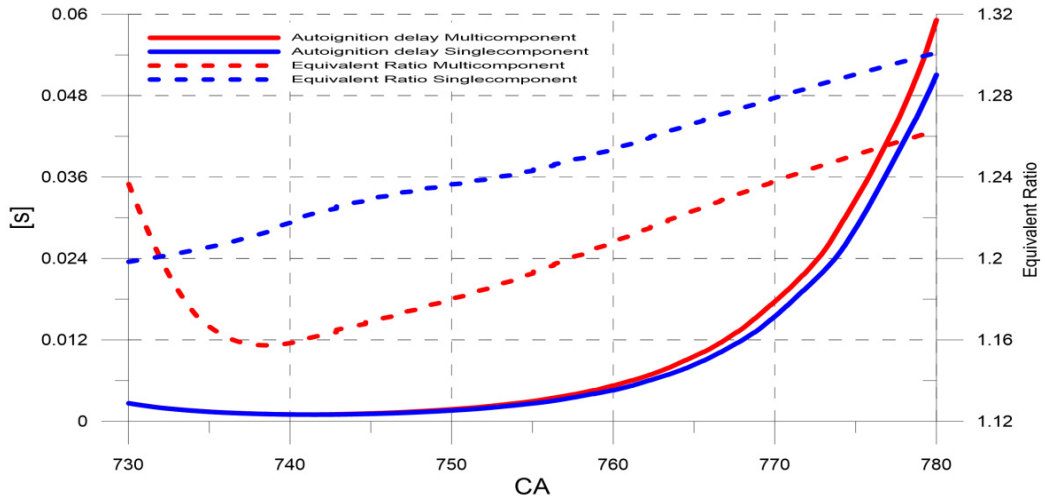

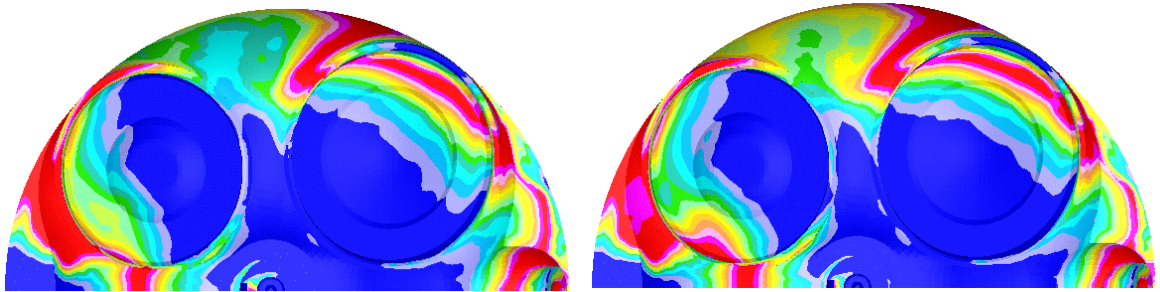Fig. 11. Autoignition delay and equivalence ratio at the exhaust sensor.

Fig. 12. Flame front at 754 CA. Multicomponent case on the left vs single component case on the right.

5. Conclusion

The study has proved that the use of a multicomponent DCMC blend instead of a standard single component fuel has a strong influence on several aspect such as fuel distribution, flame front propagation and temperature field, parameters who strongly influence both combustion and knock tendency.

Multi-component evaporation differs significantly from that of a single-component fuel in terms of the time histories of their respective evaporation rates and droplet life times. The present DCMC fuel evaporation model for multi-component sprays predicted different distributions of liquid droplets and fuel mass fractions to those from the corresponding single-component fuel. The critical area near the exhaust valve results therefore cooler in the multicomponent case and presents a richer mixture which indicates a greater autoignition delay and a not knocking behaviour also because of a slightly different flame front propagation.

The differences outlined prove that the multi-component approach can be a meaningful part of the knock tendency/combustion study since the single-component fuel behaviour cannot take into account the mutual impact on the evaporation of the different fuel components providing an excessively faster and not realistic droplet evaporation.

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