

Simulation and Optical Diagnostics to Characterize Low Octane Number Dual Fuel Strategies: a Step Towards the Octane on Demand Engine

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ABSTRACT

Reduction of CO₂ emissions is becoming one of the great challenges for future gasoline engines. Downsizing is one of the most promising strategies to achieve this reduction, though it facilitates occurrence of knocking. Therefore, downsizing has to be associated with knock limiting technologies. The aim of the current research program is to adapt the fuel Research-Octane-Number (RON) injected in the combustion chamber to prevent knock occurrence and keep combustion phasing at optimum. This is achieved by a dual fuel injection strategy, involving a low-RON naphtha-based fuel (Naphtha, RON 71) and a high-RON octane booster (Ethanol, RON107). The ratio of fuel quantity on each injector is adapted to fit the RON requirement as a function of engine operating conditions. Hence, it becomes crucial to understand and predict the mixture preparation, to quantify its spatial and cycle-to-cycle variations and to apprehend the consequences on combustion behavior - knock especially. Therefore, experimental and numerical work were conducted on different dual-fuel strategies involving Port Fuel Injection, Lateral Direct Injection and Central Direct Injection. Tests were conducted on an optical single-cylinder engine to characterize mixture preparation and combustion behavior. A semi-quantified 2-color Laser Induced Fluorescence technique was used to evaluate each fuel concentration in the chamber during the mixing process, and high-speed color imaging was performed for visualizing ignition and soot phenomena. 3D RANS simulations with ECFM combustion model were carried out showing good agreement with experimental results. Aside this validation aspect, the computations serve as numerical diagnostics to study spray to aerodynamics interactions regarding the different injection strategies and the subsequent effects on mixture formation and on the combustion. Thus, little interaction among sprays is observed, leading to a fuel distribution in the chamber driven by injectors independently. Also, regarding the operating and the inherent octane requirement, it is shown how the dual injection strategy can be adapted to maximize the anti-knock capacity of the overall fuel mixture.

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INTRODUCTION

The world's demand for energy is forecasted to grow by more than 25% in the 2015-2040 period [1, 2, 3, 4]. In the same trend, demand for transportation fuel is continuously increasing, especially in countries not member of the Organization for Economic Co-operation and Development (OECD). Projections of 1.1% worldwide annual growth are forecasted for example by the US Energy Information Administration [3] for the 2010-2040 period. As evidenced in [Figure 1](#) and [Figure 2](#), even with the emergence of alternative fuels (i.e. other than Diesel and Gasoline for road transportation, and Jet for aviation), mainly driven by light-duty vehicle fleet, fossil fuels will remain the main source of energy for transportation in the decades to come. Also shown in [Figure 1](#) is the imbalance between total volumes of gasoline and diesel fuels. Demand for diesel is mainly driven by the commercial activities that are consuming middle and heavy distillates (kerosene, diesel and marine fuels). From a refining perspective, this increasing demand of heavier fuels is a major issue. Indeed, existing infrastructure is not adapted to meet the projected

shift in fuel demand toward heavier distillates and considerable investments need to be considered to meet the demand. In this context, increasing passenger vehicle engine efficiency to reduce fossil fuel consumption and CO₂ emission is an endeavor coherent with both the automobile's industry demand and with the fuel refining industry processes.

Motivated by the existing energy landscape and outlooks, and with the initiative to promote a responsible use of petroleum products in the transportation sector, Saudi Aramco is pursuing collaborative research programs with IFP Energies nouvelles to develop and prove novel fuel/engine solutions, capable of challenging modern technological and environmental issues. One of the research initiatives uses naphtha-based fuels to power spark ignition (SI) engines, today operated on conventional gasoline. Naphtha is a generic term designating the fraction of crude oil boiling within the 30-180 °C range. It is composed of C5 to C11 hydrocarbons and has a low research octane number (RON) value, roughly within the 30-70 range. It is a refinery product

that could potentially be beneficial to the automotive industry as a low-processed fuel emitting less CO₂ during the refining process. Moreover, thanks to its higher hydrogen to carbon ratio than standard gasoline, burning naphtha in engines produces less CO₂ per unit of energy injected. Burning naphtha based fuel may lead to -4 to -7% (depending on naphtha's composition and its RON value) lower CO₂ emissions compared to standard gasoline [5].

Global transportation demand by fuel

MBDOE

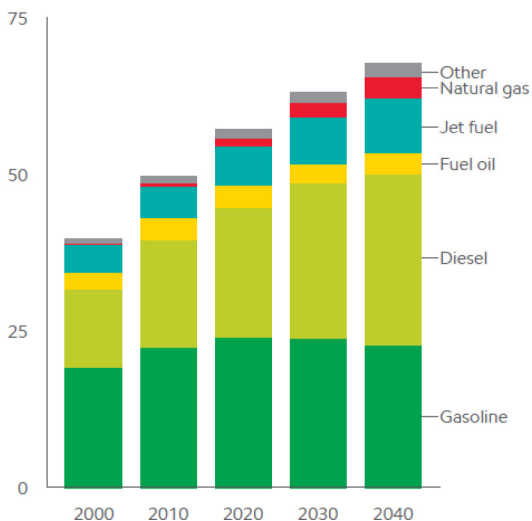
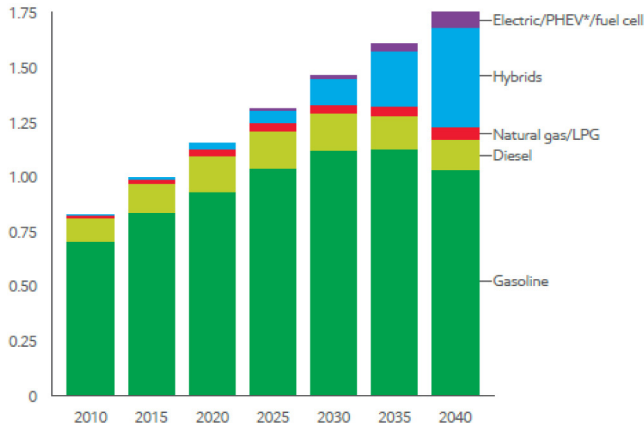


Figure 1. Projected global transportation demand by fuel, from Exxon Mobil. [1]. (MBDOE: Million Barrels per Day Oil Equivalent)

Light-duty vehicle fleet by type

Billions



*Plug-in hybrid electric vehicles

Figure 2. Projected global transportation demand by fuel for light-duty vehicles, from Exxon Mobil. [1] (y-axis: billion units)

Octane quality (which can be described by RON) of the fuel is crucial to avoid knock phenomena. In absence of knock, the combustion phasing of a spark ignited (SI) engine could be tuned in the optimal way whatever the engine speed and load conditions. This is all the more true in case of turbocharged SI engines, whereas its requirement at low load is optional. Using fuel's RON as one of the control parameters and varying RON with engine load demand gives birth to the concept *Octane on Demand*. It is a dual fuel concept in which the engine operates on a low RON base fuel for the majority

of the time and when the need of high RON arises (high load) octane booster [6, 7] is added. This way, the waste of RON can be avoided when it is not required.

On a conventional combustion engine, the change of fuel properties, especially the RON value, and its effects on engine response is being studied for several years [8, 9, 10, 11, 12, 13]. The increasing literature work indicates that this is becoming a great opportunity for car manufactures to further decrease average fleet consumption and tailpipe greenhouse gas (GHG) emission levels [6, 7, 12, 14, 15, 16, 17]. Indeed, unlocking RON value is a key parameter for enabling novel engine design. Higher compression ratio can lead to better engine efficiency at low loads without any knock limitation at higher loads due to high RON value of the fuel. Besides, high RON streams (> 105) are commonly obtained with ethanol blends or from refinery products rich in aromatic molecules (reformate). Worldwide legislations impose some bio-source content in the fuel: e.g. max. 3.7%_{molar} oxygen and max. 10%_{vol.} ethanol for EN 228 SP95 E10 European gasoline. Oxygenates are then increasingly blended in the gasoline pool to both upgrade the RON and comply with legislation. However, oxygenates have a low lower heating value (LHV) compared to non-oxygenated fossil fuels (approx. -30%). Then, the mass fuel consumption of the engine is permanently burdened by the penalty coming from the low LHV of oxygenates. In a dual-fuel approach, the minimum required oxygenate amount is used to adjust the RON *on demand*. As a result, optimum combustion phasing can be kept, ensuring optimal engine efficiency, including at full load, so that total mass of consumed fuel can be optimized. (Note that even with premium gasoline, in addition to the waste of RON at low loads, spark retard is still necessary at high load for turbocharged engines).

The present work aims at progressing in proving the feasibility of the octane on demand (OOD) concept. Based on previous works [18, 19, 20, 21], the objective is to understand mixing process with port fuel injection (PFI) and direct injection (DI) which will later help in choosing injection configuration for both base fuel and octane booster to minimize both CO₂ emissions and octane booster consumption, which is considered as a high value product. In previous work, it was shown that:

- Based on CFR (cooperative fuel research) engine measurements, Rankovic et al. [18] identified experimentally how the RON of a base-fuel plus an octane booster evolves as the octane booster ratio increases. Two low RON base-fuel (RON 71 and RON 91) and four octane boosters were tested (ethanol, refinery reformat, a mixture of di-isobutylenes (DIB), 2-butanol, and a mixture of butanols (patented Saudi Aramco stream, SuperButol™)¹. Main result was that ethanol shows interesting octane-booster properties, with a non-linear effect with respect to volume incorporation. Consequently low-RON naphtha-based fuel (RON 71) demonstrated an interesting potential: starting from RON of 71, an addition of 30%vol. of ethanol is able to match the RON 95 value of commercial gasoline.
- In [19], Bourhis et al. characterized the octane requirement of a 1.6L turbocharged direct injection (DI) multicylinder gasoline

1. Note that among the possible bio-sourced oxygenated boosters (ethanol, butanol, etc.), which could be used, it was decided in this study not to evaluate methanol for toxicity reasons of methanol, and because it is already studied by Kai et al. [22].

engine for three different compression ratios (7.5, 10.5 and 12:1), using TRFs (Toluene Reference Fuels) within a 71-111 RON range. It was shown that RON 71 could be used on a significant part of the engine map even at CR 10.5:1 keeping optimum combustion phasing without knock up to approx. 5bar BMEP (Figure 3). On top of that, non-linearity of RON requirement against engine load was observed. As a promising result, RON 71 fuel is expected to be used in significant proportion on Worldwide harmonized Light vehicles Test Procedure driving cycle (WLTP). This work enabled to define CR 10.5:1 as the best CR for this OOD concept. This resulted as a compromise among theoretical efficiency, RON requirement and brake efficiency (for CR 12:1, combustion speed was affected by the shape of the piston).

- In the work presented in [20] by Bourhis et al., real octane boosters (based on Rankovich et al.'s ones [18]) were evaluated and compared to TRFs. RON 71 naphtha-based was used as a base fuel. CR was 10.5:1 and fuels were splash-blended in single fuel GDI configuration, 1.6L multicylinder engine. Once again, ethanol proved to be a very good octane booster for its high RON, its high latent heat of vaporization (Lv) and favorable sensitivity (S=RON-MON). Interestingly, RON71 - ethanol blends showed higher knock resistance than the corresponding TRF. This is driven by the differences in Lv and S of this real fuel compared to TRF. As a result, nearly ideal conditions (according to [11]) were obtained: low-S fuel at low load, high-S at high load, and a significant "cooling effect" due to the high Lv of ethanol. Optimum combustion phasing could be maintained on the whole engine map, including at full load, and without any fuel enrichment need.
- Finally, Bedon et al. [21] performed 0D driving cycle simulations for an M-segment vehicle. Based on the steady state results from [20], this work enabled to assess the potential of Tank-to-Wheel CO₂ emissions of the OOD concept for various cycles, fuels and engine configurations. Indeed, RON 71 and RON 91 were tested as a base fuel; four octane boosters (ethanol RON 108, reformat RON 111, DIB RON 104, and SuperButol™ RON 107) were considered; and three CR (7.5, 10.5 and 12.5:1) were evaluated. Results confirmed that CR 10.5:1 enables lowest CO₂ emissions, together with the naphtha-based RON71 base fuel. Ethanol is the octane booster that minimizes both CO₂ emissions and booster consumption. This work enabled to select the optimum configuration [CR 10.5; naphtha-based fuel RON 71 as the base fuel; ethanol as the octane booster] and predict 4.6% CO₂ benefit as compared to regular E5 RON95 gasoline on the WLTP driving cycle.

All of these previous works considered pre-mixed blends of fuel in a single-fuel configuration (GDI). Along with its companion paper [23], the aim of the present work is now to evaluate the OOD concept in a dual fuel approach PFI + GDI. In addition to the best base fuel + octane booster couple selection (to confirm previous results), impact of choice of injection strategies for base fuel and booster have on the mixture formation and hence on combustion was studied in details.

In-depth understanding of the physical mechanisms driving the in-cylinder fuel mixing is proposed thanks to extensive computational fluid dynamics (CFD) and optical diagnostics investigations.

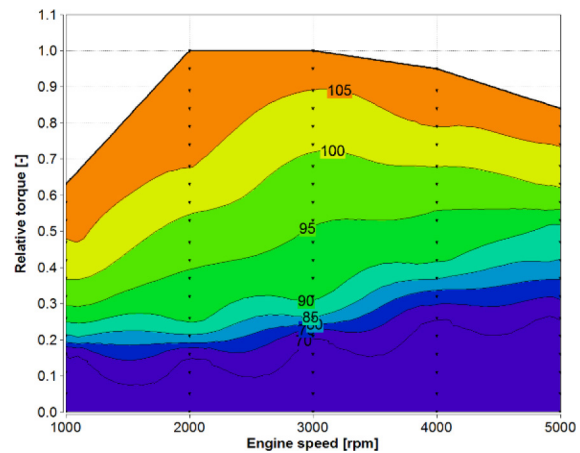


Figure 3. RON requirement at CR 10.5:1 (stock configuration).

In our knowledge no 3D CFD simulation works on OOD concept have been published. All the previous simulation works on OOD concepts mainly involves life cycle assessment, fuel consumption gain, emission reductions etc. using 0D simulations tools. The existing published 3D simulations works on dual fuel concept is mainly oriented to understand diesel-CNG combustion and then few to investigate diesel-gasoline coupling, trying to understand combustion and no detail study of mixture formation mechanism with dual direct injection and its impacts exists.

EXPERIMENTAL APPARATUS

Optical Single-Cylinder Engine

The single cylinder optical engine used in this program is a prototype designed at IFP Energies nouvelles. It is representative of a modern downsized engine with a high level of turbulence. The tumble motion was characterized using an in-house methodology and evaluated to 1.5. The engine has a capacity of 400 cm³, and a reference compression ratio (CR) of 10.5:1. This engine is equipped with an extended (bowditch) piston for optical access, though this access was not necessary in these experiments. Dry lubrication is used, meaning there is no oil film on the liner. Finally, to allow a lateral access through a 20mm-high transparent crown, the first piston ring has been lowered at 24mm from the top of the piston. Main characteristics of the engine are summarized in Table 1.

Two piston geometries were used allowing to change the compression ratio. The reference configuration corresponds to a CR of 10.5:1. A higher CR case was studied, 12:1.

Most of the experiments were conducted in motored conditions though some combustion tests were performed. In all combustion cases, the spark advance (SA) is fixed at 10°CA BTDC (crank angle before top dead center).

Table 1. Engine main characteristics.

	IFP Energie nouvelles prototype optical engine
Type	Single cylinder, 4 valves
Capacity	400cc
Bore x Stroke	77 x 85.8 mm
Compression Ratio	10.5:1 & 12:1
Flow motion	Tumble 1.5 (steady-flow rig characterization)
Fuel	Isooctane

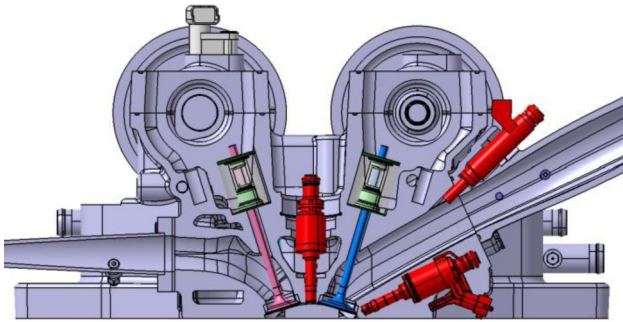


Figure 4. 3D sketch of the cylinder head showing the different injection strategies.

Injection Strategies

Three injection geometries were used on this engine. Figure 4 shows the localization of the injectors.

- A port-fuel injector can be mounted in the intake port close to the intake valves. The injector used is a Bosch EV6B. The typical injection pressure is 5bar.
- A central direct injector can be mounted using a 5-hole HDEV-5.2 Bosch injector with a typical injection pressure of 200bar.
- A lateral direct injector can be mounted next to the intake port. The injector used is a Bosch HDEV-5.1 with a typical injection pressure of 105bar.

Thus, different injection strategies are possible. Single injection was performed using each injector separately. Dual injection was performed using the two direct injectors, with the possibility to vary the injected fuel quantity ratio between the injectors. Figure 5 shows sprays patterns from the two direct injection strategies

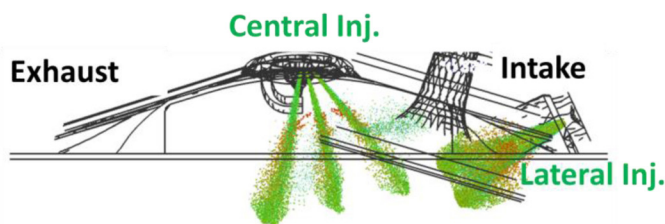


Figure 5. Lateral and central direct injection targeting (spray patterns, from 3D calculations).

Optical Accesses

To allow visualization inside the combustion chamber, the optical single-cylinder engine is configured with several optical accesses. Quartz windows are mounted in the cylinder head to allow access to the vicinity of the spark plug to characterize the early stage of combustion (Figure 6).

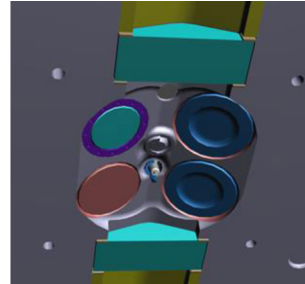


Figure 6. 3D sketch of the cylinder head mounted with quartz windows.

For mixture preparation characterization, a full transparent liner made of sapphire was used. For combustion characterization, a sapphire crown of 20mm height mounted between a full metal liner and the cylinder head was preferred (Cf. Figure 7). This configuration leads to relocate the first piston ring below the transparent liner when the piston is at top dead center (TDC).

Optical Diagnostic for Mixture Characterization

The aim of this work is to understand the mixing process during a dual fuel injection. Therefore, a methodology to track each fuel independently and simultaneously is required. Laser Induced Fluorescence (LIF) is a well-known and efficient method to measure fuel concentration in a combustion chamber [23]. An evolution of this methodology is the two-tracer LIF technique that was used [24, 25]. It consists in using two different tracers (each injected from one of the dual fuel injectors) emitting an induced fluorescence signal, each at a specific wavelength, with very little interference at the others'. Also, the base fuel has to be non-fluorescent. Therefore, isooctane was chosen as a good gasoline surrogate with no induced fluorescence. The two tracers were α -methyl-naphthalene (1MN) and toluene. They were chosen because of their high level of quantum yield efficiency, and their very little interference in emission spectra [26]. The concentration of tracer in fuel was 0.05% for 1MN and 0.5% for toluene. The assumption was made that the two tracers were sufficiently co-evaporant to isooctane, in order to guarantee good representativeness of the tracer local concentration.

The two-tracer LIF technique was achieved using a frequency-quadrupled Nd:YAG laser (266 nm). As shown in the schematic of Figure 7, a laser sheet was formed using a cylindrical & spherical doublet producing a laser sheet of 20mm in height and less than 2mm in thickness. Fluorescence 2D signal was then collected through the transparent crown by two ICCD (intensified charge-coupled device) cameras (Princeton PI-Max) arranged on both side of the laser sheet. Each camera was mounted with an optical band pass filter corresponding to each tracer respectively. The camera gate (exposure) time was maintained constant at 150 ns for all LIF experiments as

this was found to provide satisfactory tracer LIF image signal-to-noise ratio whilst allowing sufficient margin for any potential camera/laser timing jitter.

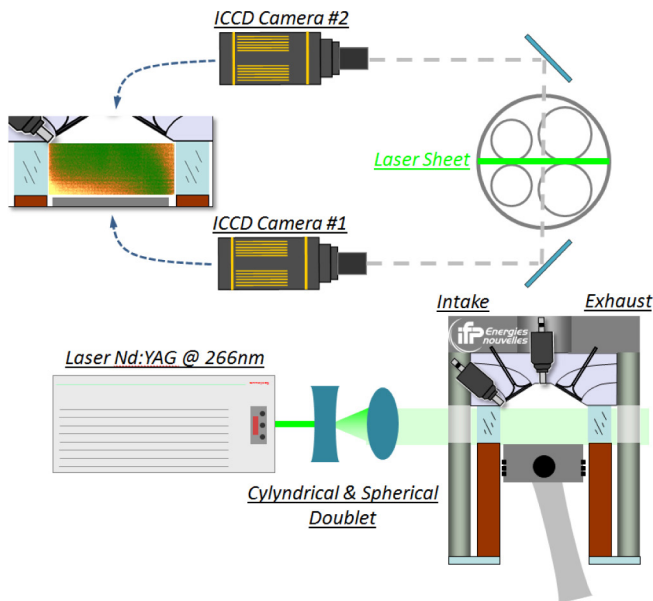


Figure 7. 2-tracer LIF setup on optical engine.

A specific protocol of acquisition was set to ensure accuracy and repeatability. One LIF acquisition per cycle was performed at 60°CA BTDC. This timing ensured a maximum field of view in the chamber through the transparent crown. One hundred cycles were recorded per operating points, which were repeated three times. Overall, it represents three hundred instantaneous LIF images per operating point. This ensured a good convergence when averaging these images. The cycle-to-cycle spatial variability was evaluated at 10% on 10mm² area for each operating points. No significant difference between operating points was observed.

Images from ICCD camera #2 were horizontally flipped so that each image presented in this paper looks like the one taken from the same side of the engine. Therefore, the intake side of the engine is on the left side of LIF images and the exhaust side on the right side, as shown in Figure 7. The location of the image plane is as shown in Figure 7, i.e. in the center of the chamber. The images presented in the paper take into account a margin of approximately 1mm from the wall to avoid light aberration.

A calibration method was developed to infer local fuel-air equivalence ratio (FAER) in the plan of the laser sheet. The calibration was realized by injecting known quantities of tracer through port fuel injection. The calibration protocol allows to infer the fuel-air ratio by type of tracer. A post processing protocol was then applied to each image to take different sources of error into account. First, each image is normalized by the energy of each laser pulse. A flat field correction is then applied. Hypothesis is made that all the fuel is completely vaporized. Thus if liquid fuel is still present at the measuring timing, the overall FAER should be corrected. This correction was not made since the main purpose of this work is to compare the influence of the injection strategies. Furthermore temperature influence on the fluorescence signal was not taken into

account other than assuming the conditions of calibration and FAER characterization are similar. Therefore this calibration method can be considered as semi-quantitative.

Figure 8 shows examples of post-processed images obtained for the CR10.5:1 single fuel, side and central injections operating point (L100 & C100 in Table 3). On the top two images, we compare the average measurement of the fuel injected through the lateral injector on the two cameras. On the bottom two images, we compared the results obtained with a single central injection. Thus we demonstrate the good selectivity of our optical filtration strategy for each tracer.

The overall equivalence ratio not being equal to one is explained by several factors. First the planar LIF measurement is a 2D measurement. Thus it does not take into account the fuel outside the laser sheet, located in the center of the chamber. Moreover, as mentioned earlier, the calibration method is not totally quantitative. Therefore some parameters are not taken into account that could modify the overall FAER estimation, such as local temperature, pressure, oxygen content.

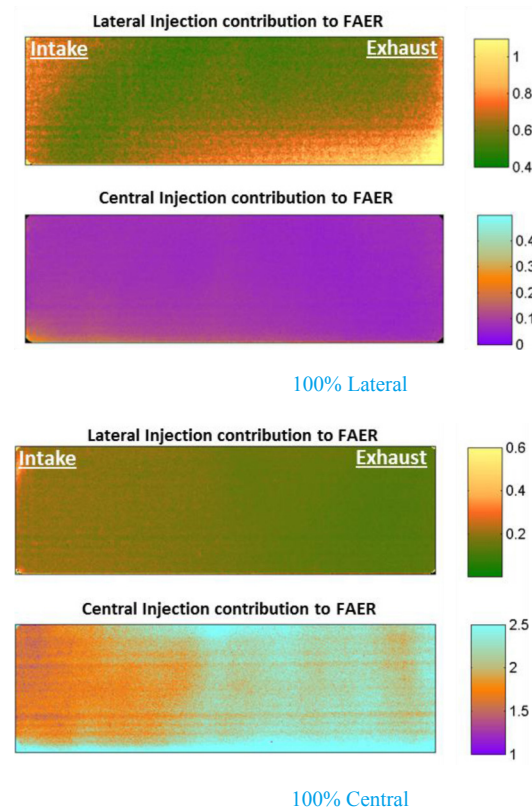


Figure 8. LIF averaged images taken at 60°CA BTDC for single injection strategies, 100% lateral (L100) & 100% central (C100). For each strategy the image on top represents the fuel injected through the lateral injector, and the bottom one the fuel injected through the central injector.

Operating Points and Test Matrix

This paper presents the results obtained with a single engine operating condition - 1200rpm x 8bar IMEP (indicated mean effective pressure) in stoichiometric conditions. The settings are given in Table 2. Mixture characterization was done using surrogate fuel (isooctane) in motored conditions. To avoid LIF signal quenching issues, fuel

oxygen, nitrogen was preferred to operate the engine. Since at this point no combustion is needed, nitrogen is considered to be equivalent to air.

Table 2. Operating point settings

Engine speed	1200rpm
Load	8bar
In flow rate	11.3kg/h
Intake Pressure	0.926bar
Intake Temperature	35°C
Start of Injection	260°C A BTDC

Single and double injection strategies were studied. For double injection strategies, different ratios in injected quantities were studied. Table 3 resumes all the injection strategies that were considered. The percentages are related to injection duration. As a reference the duration of operating points L100 and C100 are 2.1ms and 2.2ms respectively. Each point was operated for CR10.5:1 and CR12:1.

Table 3. Test Matrix for two-tracer LIF experiments.

	Port	Lateral	Central
P100	100%	0%	0%
L100	0%	100%	0%
C100	0%	0%	100%
P25L75	25%	75%	0%
P50L50	50%	50%	0%
P75L25	75%	25%	0%
L75C25	0%	75%	25%
L50C50	0%	50%	50%
L25C75	0%	25%	75%

SIMULATIONS SETUP

The goal of the numerical work presented here is to study spray to aerodynamics interactions to help design a flexible OOD engine concept. Therefore it was chosen to run the calculations in conditions close to the targeted engine conditions. Thus instead of iso-octane, fuels of primary interests for the OOD project were used: naphtha and ethanol. In the same way, simulations were performed in combustion mode whereas experiments were performed in motored conditions due to optical engine limitations. These main differences between experiments and simulations are significant and will be discussed through the results section.

Thus several operating conditions studied with the optical test bench engine described above were also studied using RANS 3D CFD computations. Indeed, operating points at CR10.5 were simulated in order to bring additional information to help understand the physical phenomena involved in the OOD concept - mixture preparation, interactions between injections and air-motion, auto-ignition *etc.*... The three different injection strategies were simulated in mono and dual injection configurations.

3D CFD computations were performed with the IFPEN 3D CFD solver [23]. This code is a hybrid mesh unstructured parallel (MPI) solver for reactive compressible gas flows with sprays dedicated to multi-physics, three-dimensional simulations. It is dedicated to the computation of reactive flows in internal combustion engines, solving the RANS (Reynolds-averaged Navier-Stokes) equations using a finite volume method extended with the Arbitrary Lagrangian Eulerian (ALE) algorithms. The code uses the well-known time splitting decomposition. The temporal integration scheme is largely implicit. Species (and tracers), energy and the RNG k- ϵ turbulent diffusion terms are implicitly solved by a generic diffusion routine. The convection terms are explicitly subcycled. A second order upwind scheme for scalar and momentum convection is used. Several in-house detailed physical models are available in this CFD tool. In the present study, dealing with SI engines, the Imposed Stretch Spark Ignition Model (ISSIM) [31] based on an Eulerian approach of a flame density transport equation is used to model spark ignition. Instead of resolving the spherical kernel equation 0D way, ISSIM directly uses it in the Eulerian transport equations, therefore allowing a local description of all phenomena. The subsequent combustion is modeled using the Extended Coherent Flame Model (ECFM) [29]. The ECFM model is based on the resolution of a transport equation for Σ (flame surface density). In the model each cell is divided in two zones: the burnt gas zone and the fresh gas zone. These zones have separate local combustion related variables. Tabulated Kinetics of Ignition (TKI) model is used for auto-ignition detection [30]. Turbulence modeling is performed with the k- ϵ RNG model [32] while the law-of-the-wall is computed according to the model of Kays and Crawford [33]. Decades of experience of SI engine CFD simulations governed choice of these models. Test of different other possible models were not carried out in the present work.

Spray description relies on a Lagrangian model accounting for spray atomization (wave model) and break-up (FIPA model) [34]. Starting with standard gasoline engine injector parameters, spray cone angle, droplet size (represented by Sauter mean diameters (SMD)), and FIPA constant were calibrated to fit the experimentally-observed spray dynamics in a test cell. The test cell pressure and temperature was chosen based on the average pressure and temperature found in the cylinder during injection. As injection happens during intake phase, pressure and temperature in the cylinder does not evolve during the injection. So the calibrated injection parameters remains valid for all the tested engine points.

Specificities of all the different fuels considered in the present study have to be taken into account in the numerical model.

Thermodynamic fuel properties were generated using ReFGen, [35] in order to well represent the injection related phenomena and the vaporization. ReFGen models the fuel as few pseudo-components ($C_xH_yO_z$) characterized by their molecular weight, critical properties and acentric factor taking into account the distillation curve and density of the fuel. Moreover, each fuel laminar flame speed (S_L) correlation was chosen among the correlations available in the code in order to well represent the flame development during combustion. Respecting distillation curve, composition, RON and MON of the fuel, surrogates of all the fuels were generated using Chemkin-pro. Finally, a specific auto-ignition delay table was built for each of the