Fuel Sensitivity effects on Dual-mode Dual-fuel Combustion Operation for Different Octane Numbers

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Abstract

The dual-mode dual-fuel combustion is a promising combustion concept to achieve the required emissions and carbon dioxide reductions imposed by the next emissions standards. Nonetheless, since the combustion concept relies on the reactivity of two different fuels (diesel and gasoline), the fuel formulation requirements are stricter. This work investigates the effects of the low reactivity fuel sensitivity for different octane numbers at different operating conditions representative of the combustion regimes found inside the dual-mode dual-fuel engine map. For this, experimental evaluations were performed using fuels with research octane number 92.5 and 80 and different sensitivities (0, 5 and the maximum one achievable for each fuel). The combustion development was assessed by means of the heat release rate characterization. Moreover, numerical simulations in a constant volume homogeneous reactor were used to explore and understand the impact of the different fuels on the ignition delay time. The results suggest that the sensitivity increase affects the different research octane number fuels in a different way. For the fuel with research octane number 92.5, the sensitivity variation increases the experimental ignition delay, impairing the combustion

process and increasing the fuel consumption. In the case of the fuel with research octane number 80, the sensitivity increase does not affect the combustion development. This was justified by the numerical investigation, which points to a wider temperature range where the sensitivity does not affect the final ignition delay for research octane number 80. Moreover, generally, the ignition delay times for research octane number 80 considering the experimental gasoline fraction used are half than those of research octane number 92.5. At full load conditions, the trend is inverted, where the experimental ignition delay for research octane number 80 is affected by the sensitivity whilst research octane number 92.5 presents only modifications after the combustion start.

Keywords

Dual-fuel combustion; fuel sensitivity, octane number; ignition delay; reactivity-controlled compression ignition

1. Introduction

The regulations that limit the main pollutants emitted by the internal combustion engines act as a driven force for the development in this field of the technology [1]. It is expected that the next normative will require reductions of 15% in the total carbon dioxide (CO_2) emissions produced by the internal combustion engines in medium- and heavy-duty applications to 2025 [2]. Since the amount of CO_2 emissions is proportional to the fuel consumption, the improvement of the engine efficiency is a direct way to reduce this pollutant [3]. Moreover, this must be accomplished while maintaining the emissions of the other regulated pollutants at low levels [4]. While state-of-art devices to reduce the hydrocarbons (HC) [5], carbon monoxide (CO) [6] and nitrogen oxides

(NOx) emissions [7] already exist, these devices entail an additional cost to the final vehicle [8] and have negative impacts on the engine efficiency [9].

Considering this scenario, great efforts have been made to develop new combustion concepts able to provide improvements in fuel consumption and reductions on the final emissions at the same time [10]. In this field, the reactivity controlled compression ignition (RCCI) combustion can be highlighted as one of the most promising concepts [11] due to the balance between fuel consumption, emissions and operating range [12]. This concept is based on using two fuels with different reactivity [13], allowing to tailor the reaction rate by modifying the amount of each fuel [14]. This provides a greater degree of control on the combustion development compared to other low temperature combustion (LTC) concepts as the homogeneous charge compression ignition (HCCI), which relies only in the in-cylinder conditions and the reactivity of a single fuel [15]. Despite of this, the RCCI concept is still limited on the operating zone of the engine [16] [17]. As a solution, Benajes et. al [18] proposed a multi-mode combustion concept moving from a fully premixed combustion (as RCCI) at low loads towards a diffusive dual-fuel one at high loads. The multi-mode combustion concept allows the dual-fuel operation in the whole engine map; however, some calibration constraints as NOx and soot emissions must be relaxed [19]. Additionally, as the combustion strategy shifts towards to a diffusive one, the engine efficiency decreases as a consequence of the higher combustion duration [20]. Therefore, during the engine calibration it is intended to obtain the maximum percentage of the engine map operating with a premixed combustion. To achieve this, a deep understanding about the combustion process and the governing parameters as the fuel properties, in-cylinder composition, temperature, pressure, etc. is required.

The chemistry involving the dual-fuel combustion is complex as it presents the combination of different fuels with contrasting characteristics, as for example diesel and gasoline. The properties of each one have a fundamental role on the combustion progress. In the case of the gasoline, properties as the octane number and the sensitivity, defined as the difference between the research octane number (RON) and the motor octane number (MON), are widely used as measures to qualify the fuels regarding its auto ignition potential [21]. In particular, the sensitivity (S) has a major impact on specific ranges of temperatures and pressures, and it is related to the fuel composition [22]. Leppard carried out a significant contribution on the understanding of the fuel octane origins [23]. Applying a cooperative fuels research (CFR) engine, he evaluated several paraffins, olefins and aromatics at different operating conditions [24]. The results demonstrated that the paraffinic auto-ignition is dominated by negative temperature coefficient (NTC), being more pronounced at higher temperatures and lower pressures. Olefins and aromatics did not present a NTC during the investigations. In this sense, two categories of fuels were defined: sensitive and non-sensitive fuels. The first category addresses the fuels that does not present NTC region whilst the second are affected by the low temperature heat release from the NTC region, resulting in reduced octane quality at motor rating conditions.

A special effort was done to identify surrogates that allow to tailor the sensitivity of the blend that allow to emulate the behavior of multi component commercial gasoline [25]. Whilst octane and heptane blends have been demonstrated to work as surrogate for gasoline in some conditions, generally, it is needed an aromatic compound to add sensitivity to the mixture. The commercial gasoline contains a high concentration of aromatics, presenting high concentrations of toluene (up to 35%). Therefore, it was

suggested the addition of this component to the mixture to allow to adjust the C/H ratio and the ignition characteristics [26]. Gauthier et al. demonstrated by means of shock tube evaluations that ternary blends containing n-heptane, isooctane and toluene (20%v/v of toluene) can reproduce the ignition characteristics of a multi component commercial gasoline [27]. Different chemical kinetic mechanisms have been developed to properly describe the combustion of these ternary blends [28]. Mehl et al. [29] developed an approach for formulating surrogates for gasoline with application towards a reduced surrogate mechanism for CFD engine modeling considering a limited set of information of the real fuel. The use of composition and parameters as the sensitivity, anti-knock index (AKI) and the slope of the NTC region provided important insight for the surrogate formulation and mechanism reduction. As a result, the detailed mechanism used as start point could be reduced to about 300 species while maintaining the predictive capability regarding ignition and combustion parameters.

In the light of this, several evaluations were carried out in order to identify the impact of the sensitivity in different combustion devices representing conditions found in internal combustion engines [30]. Westbrook evaluated the chemical kinetics of the octane sensitivity in a spark ignition engine by means of a chemical Kinect modelling for 1-alcohols, linear olefins, and n-alkyl benzenes [31]. The results allowed to determine the pathways responsible for the absence of the low temperature reactivity, being attributed to the electron delocalization, which follows different paths in each class of high octane sensitivity fuel. Ignition studies were performed by Javed et al. [32], aiming to provide a database for the mechanisms development and understand the impact of RON and sensitivity on the ignition process for different RON and sensitivity fuels in a high pressure shock tube and in a rapid compression machine. The results from

experiments were compared to those obtained by simulation using the Lawrence Livermore National Laboratory (LLNL) mechanism [33]. Despite of the deviations from the current Kinect mechanism, it was verified that the NTC region was more pronounced for low RONs, low sensitivity fuels due to the higher production of hydroperoxil radical (HO_2) and hydrogen peroxide (H_2O_2). The underlying sensitivity phenomena that impacts the combustion development in advanced compression ignition concepts were addressed by Tao et al by means of numerical investigations in a HCCI model developed in Chemki-Pro [34]. The numerical investigations allowed to state that even fuels with similar octane ratings can present noticeable differences in its behavior. Moreover, it was also reinforced the significance of the sensitivity on the HCCI condition, mainly on zones where NTC affected regimes are presented. Hellier et al. [35] evaluated different toluene/heptane blends in a direct injection compression ignition engine to identify the effects of the binary mixture on the combustion phasing and exhaust emissions. The increase in the toluene quantity impaired the ignition quality of the mixture. For concentrations higher than 50% toluene by volume in the mixture, no ignition was verified.

Despite of the relevant information found in the literature, there are no specific studies addressing the impact of the sensitivity variation in dual-mode dual-fuel combustion operating with diesel and gasoline. In this sense, the aim of this study is to investigate the effects of the sensitivity on the combustion process at different octane numbers by means of experimental tests in a multi-cylinder engine modified to operate under dual-mode dual-fuel combustion. A ternary blend of isooctane, n-heptane and toluene was used as surrogate of gasoline to realize different sensitivities. Three different sensitivity values (0, 5 and the maximum achievable) were evaluated at two different research

octane number (92.5 and 80). Three operating conditions were chosen to assess the impact of the mixtures to provide insight about the influence of the temperature and pressure conditions on the combustion process of the different fuels. Moreover, detailed chemical kinetics evaluations were performed in the package Cantera for specific operating conditions to determine the behavior of the different sensitivity on the mixture reactivity.

2. Materials and methods

This section describes the main characteristics of the test cell used in this study, focusing on the engine unit and the different systems of which is equipped. Moreover, the main properties of the fuels used in the present investigation are detailed here. Finally, some considerations about the procedure followed during the experimental tests and the bases of the theoretical tool used to perform the chemical kinetic calculations are provided.

2.1. Engine characteristics

The main characteristics of the engine used during the investigation are presented in Table 1. It consists of a multi-cylinder platform, medium-duty, four stroke, serial production 7.7L engine. The geometry of the piston used in this engine was optimized in previous works using a single-cylinder version of this engine platform together with computational fluid dynamics (CFD) [36]. In this sense, the original geometric compression ratio was reduced from 17.5 to 12.75:1. This was done aiming to realize full load operation with dual-fuel combustion, reducing the mechanical demand at high load conditions. Moreover, the bowl shape was also optimized to improve the combustion efficiency and reduce the heat transfer.

Table 1. Main engine characteristics.

Engine Type	4 stroke, 4 valves, direct injection
Number of cylinders [-]	6
Displaced volume [cm^3]	7700
Stroke [mm]	135
Bore [mm]	110
Piston bowl geometry [-]	Bathtub
Compression ratio [-]	12.75:1
Rated power [kW]	235 @ 2100 rpm
Rated torque [Nm]	1200 @ 1050-1600 rpm

2.2. Test cell description

The engine test bench used to perform the investigations is presented in Figure 1. It consists of several measurement devices as well as sensors and subsystems to monitor, control and obtain insights about the different process of interest during the research. It includes a fully instrumentation of the engine with an instantaneous in-cylinder pressure per cylinder, which allows to verify and maintain the combustion process as similar as possible for each one of them. The combustion process was assessed by applying an online heat release analysis routine on the pressure signals. In this sense, the characteristic times as CA10, CA50 and CA90 as well as the shape of the heat release were maintained between different experiments for comparison. Moreover, additional instantaneous and average sensors were used at different locations of interest to assess properties as pressure and temperature, as shown in Figure 1.

Regarding the engine control, different devices dealt with the required tasks during the engine operation. The original electronic control unit (ECU) was used to control most of the original hardware as injection pressure, turbocharger rack position and high pressure exhaust gas recirculation (EGR). Nonetheless, the injector actuation was

overridden by signals from a specific control routine developed in LabView. This code allowed to control de injection settings of both high reactivity fuel (HRF) and low reactivity fuel (LRF) as well as to acquire, process and save instantaneous signals. Finally, this routine was also responsible to manage an additional low pressure EGR circuit. This system was installed to allow dealing with the high EGR demands of the combustion concept and to maintain a proper energy flow through the turbine, enabling to reach the desired boost pressures. The engine speed and load were controlled by means of an AVL active dynamometer using the AVL Puma interface. It consists of a fully integrated solution that besides of controlling the engine, it can acquire, process and save a huge amount of data.

The major combustion products from each operating condition were measured by different measurement devices applying specific methods for each specie. Most of them were measured by a five-gas Horiba MEXA-7100 DEGR analyzer. This device is able to obtain measurements of unburned hydrocarbon concentration by means of flame ionization detection. Additionally, the oxygen (O_2) is measured by paramagnetic principle whilst CO can be obtained from non-dispersive infrared and nitric oxide (NO) and nitrogen dioxide (NO_2) by chemiluminescence. In addition, the Horiba MEXA-7100 DEGR has an additional CO_2 measurement system allowing to measure this specie in both intake and exhaust to calculate the instantaneous EGR rate. An AVL 415S smoke meter was used to obtain the values of smoke emissions in filter smoke number (FSN) units. Three consecutive measurements of 1 liter volume each with paper-saving mode off were took at each engine operating point [37]. The accuracy of the main elements of the test cell is presented in Table 2.

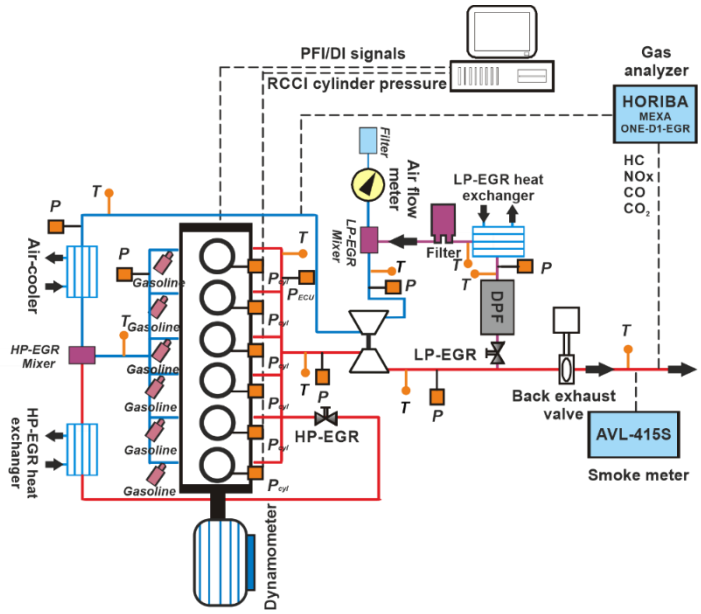

Figure 1. Configuration of the test cell used during the experiments.

Table 2. Accuracy of the instrumentation used in this work.

Variable measured	Device	Manufacturer / model	Accuracy
In-cylinder pressure	Piezoelectric transducer	Kistler / 6125C	±1.25 bar
Intake/exhaust pressure	Piezoresistive transducers	Kistler / 4045A	±25 mbar
Temperature in settling chambers and manifolds	Thermocouple	TC direct / type K	±2.5 °C
Crank angle, engine speed	Encoder	AVL / 364	±0.02 CAD
NOx, CO, HC, O_2, CO_2	Gas analyzer	HORIBA / MEXA 7100 DEGR	4%
FSN	Smoke meter	AVL / 415	±0.025 FSN
Gasoline/diesel fuel mass flow	Fuel balances	AVL / 733S	±0.2%
Air mass flow	Air flow meter	Elster / RVG G100	±0.1%

2.3. Fuels and injection systems characteristics

This subsection describes the main properties of the fuels and the injection systems used in the present investigation.

2.3.1. Fuels

Among the different components that can be used to tailor the fuel sensitivity, the use of toluene is one of the most common methods due to its properties as solubility in a wide range of components. Therefore, toluene, isooctane and n-heptane were mixed at different ratios to obtain the low reactivity fuel blends to be tested. The characteristics

of each component are presented in Table 3. It is worthy to note that EN 590 diesel was used as high reactivity fuel.

Table 3. Physical and chemical properties of the fuels and singular components used to obtain the blends.

	EN 590 diesel	n-heptane	isooctane	Toluene
Density [kg/m^3] (T= 15 °C)	842	645	658	866
Viscosity [mm^2/s] (T= 40 °C)	2.929			
RON [-]	-	0	100	121
MON [-]	-	0	100	107
Cetane number [-]	51	-	-	
Lower heating value [MJ/kg]	42.50	44.57	44.43	40.59

The different sensitivities and octane numbers were obtained following the procedure described in [38]. The final composition of each mixture used in the present work is presented in Table 4. All the blend properties as lower heating value and density were calculated from ponderations according to the mass fraction of each one of the singular components. Three different sensitivities were tested for each RON; 0, 5 and the maximum one achievable according to the RON. The limitation in the sensitivity values are presented in [38], were a plateau is obtained as the sensitivity is increased.

Table 4. Mass fraction composition of each one of the fuel blends evaluated.

	TRF 92.5			TRF 80		
	S=0	S=5	S=9	S=0	S=5	S=8
Y Toluene	0.000	0.293	0.577	0.000	0.326	0.604
Y Isooctane	0.925	0.575	0.247	0.800	0.412	0.087
Y N heptane	0.075	0.132	0.176	0.200	0.263	0.309

2.3.2. Injection systems characteristics

The HRF was injected into the cylinder using the stock common-rail fuel injection system, with a centrally located solenoid injector. The gasoline fuel was port-injected by means of the port fuel injectors (PFI) located at the intake manifolds. All the injectors were handled through a DRIVVEN control system. The direct injected (DI) and PFI fuel mass

flows were measured using dedicated AVL 733S fuel balances. The main characteristics of the DI and PFI are depicted in Table 5.

Table 5. Characteristics of the direct and port fuel injectors.

Direct injector		Port fuel injector	
Actuation Type [-]	Solenoid	Injector Style [-]	Saturated
Steady flow rate @ 100 bar [cm^3/min]	1300	Steady flow rate @ 3 bar [cm^3/min]	980
Included spray angle [°]	150	Included Spray Angle [°]	30
Number of holes [-]	7	Injection Strategy [-]	single
Hole diameter [µm]	177	Start of Injection [CAD ATDC]	340
Maximum injection pressure [bar]	2500	Maximum injection pressure [bar]	5.5

2.4. Testing methodology

Three different operating conditions were evaluated during the experiments: 25%@950rpm (fully premixed), 50%@1800rpm (fully premixed) and 100%@2200rpm (diffusive dual-fuel). The chosen operating conditions cover different zones of the calibration map allowing to have a general overview of the impact of the sensitivity variation on the engine performance. At each operating condition, for the case of S=0, a calibration methodology was applied in order to find the best settings that deliver the minimum fuel consumption while maintaining NOx and soot emissions at similar levels to the calibration constraints verified during the diesel-gasoline calibration. Once the settings are obtained, they are fixed for the remaining sensitivities to isolate only the effects of the fuel sensitivity on the combustion development. Details about the calibration methodology can be found in previous works [39].

2.5. Homogeneous reactor model with detailed kinetics

As aforementioned, there is a non-monotonicity behavior as the temperature is decreased for cases where the sensitivity is near to zero. This effect is attributed to the NTC and depends on the pressure, temperature and air fuel ratio, among others.

Therefore, different behaviors can be observed for fuels with the same RON but different MON.

In general, during the internal combustion engine (ICE) operation, these effects cannot be directly visualized as a consequence of the several phenomena taking place at the same time. Therefore, controlled experiments are needed to properly highlight and evaluate the distinct behaviors of the fuels, as those carried in shock tubes, well stirred reactors, etc. Another widely used approach is the use of 0D simulations that are able to emulate the behavior of these experiments by solving detailed chemistry for mechanisms adjusted in the conditions of interest for the oxidation of the fuels studied. In this sense, it was proposed a theoretical investigation using the package Cantera [40], which has been extensively applied in the academy with several reported results [41].

For this, a homogeneous adiabatic constant volume reactor was modelled, and different boundary conditions were applied to the reactor. First, both RONs (92.5 and 80) with the different sensitivities were assessed for a specific range of temperatures and equivalence ratios, with the same initial pressure. Finally, the values of the temperature and pressure evolution during the compression stroke were applied as boundary conditions to assess the reactivity of the mixture just before the first noticeable heat release. The temperature and pressure values were obtained by means the in-house combustion analysis routine CALMEC. The ignition delay was obtained considering the maximum value of the OH radical. A detailed reaction mechanism from Andrae [42] was selected according to a previous evaluation in the work performed by Tao et al. [34], where it was demonstrated that this mechanism is able to provide the minimum error in the ignition delay prediction for engine-like conditions. This mechanism involves 137

species and 633 reactions with detailed toluene oxidation reactions. This degree of complexity allows to capture all the chemistry involving the initiation steps that define the ignition delay time of the blend.

It is important to mention that some assumptions should be made to clarify the limitations of the analysis performed in the 0-D reactor. As one of the main characteristics of the dual-mode dual-fuel (DMDF) combustion is the generation of a reactivity stratification through the high reactivity fuel injection, a 0-D analysis cannot properly represent the experimental conditions. By this reason, only some operating conditions were evaluated thought the 0D code. In particular, the conditions selected to be studied were those in which the diesel fuel was injected early in the compression stroke and in low quantities. This helps to reduce the charge stratification, approaching a homogenous compression ignition. The main assumptions used during the work are:

- The LRF is assumed to be fully vaporized and perfectly mixed inside the combustion chamber.
- The HRF injections are early enough to obtain a homogeneous mixture. Besides, the conditions evaluated should present a high level of gasoline fraction to support this assumption, since gasoline is injected at 340 crank angle degrees (CAD) before top dead center (bTDC).
- EGR is assumed to be composed of N_2 and CO_2.
- There is no temperature gradient inside the combustion chamber.
- N-Heptane is used as the surrogate of the HRF (diesel) based on literature review [43]. As demonstrated in previous studies, this surrogate fuel is able to emulate the ignition qualities of diesel [44].

- As N-Heptane is presented also in the blend in the LRF, its mass fraction is determined considering the GF values.

The unique condition that satisfies these assumption, and therefore was selected to be studied is 50% load and 1800 rpm. Therefore, the detailed evaluation through chemical kinetics is performed just for it, and the main conclusions obtained during the investigation are used to support and justify the additional experimental results.

3. Results and discussion

This section discusses the influence of the fuel sensitivity on the combustion development by combining the experimental heat release diagrams supported by different studies performed in Cantera. Finally, a comparison among the different fuels and sensitivities is presented to evaluate the final impact on the performance and emissions parameters.

3.1. Effect of the fuel sensitivity on the combustion development

The use of different RONs in the experiments required different settings to avoid problems as pressure gradients an early combustion. In this scenario, it is difficult to isolate the effects of the sensitivity. Therefore, this section presents the results of simulations for different conditions to assess the effect of the sensitivity on the combustion. First, the impact of LRF sensitivity on the ignition delay for iso settings was evaluated. Finally, the real settings regarding charge dilution and gasoline fraction were employed to evaluate the impact of these modifications on the ignition delay.

3.1.1. Impact of fuel sensitivity on mixture reactivity at fixed conditions

A detailed analysis was performed in Cantera to understand the effects of the fuel RON and sensitivity variation in a well stirred constant volume reactor. It is clear that this kind

of simulation is not able to capture all the complex phenomena that occur during the operation of an internal combustion engines. Nonetheless, it allows to decouple the effects from flow movements, temperature gradients and heterogeneities in the mixture, isolating the effects from the fuel blends evaluated. Firstly, the results of a theoretical study having the same pressure and temperature inside the combustion chamber for both fuels are presented. In this case, the CO_2 dilution level used for both fuels was near that verified experimentally, while the initial pressure was 48 bar, representative of the experimental conditions at the end of compression stroke. In these calculations, only the effect of the low reactivity was assessed, i.e., a gasoline fraction (GF) equal to 1 was used.

Figure 2 illustrates the ignition delay time behavior as a function of the initial temperature in the reactor for an equivalence ratio of 0.6. This equivalence ratio was selected considering the conditions found in the gasoline at the point 50%@1800rpm. As it was previously discussed, the different sensitivities were realized by increasing the toluene quantity up to the maximum value obtainable in the blend (9 for RON 92.5 and 8 for RON 80). From Figure 2, it can be observed the non-monotonicity for both primary reference fuels (PRF) with S=0. Nonetheless, while the RON 92.5 still has a NTC behavior for phi=0.6 at S=5, the ignition delay time of RON 80 increases almost monotonically for the same conditions. Moreover, S=5 seems to be the most affected condition as the PRF is modified, reaching similar values for low temperatures and having larger deviations at the half of the temperature range. Even in this case, it is clear that the RON 80 is always more reactive than the RON 92.5 for the same sensitivity. Nonetheless, the intersection of the different curves at the low temperature zone indicates that the sensitivity plays a fundamental role on the ignition process of the mixture.

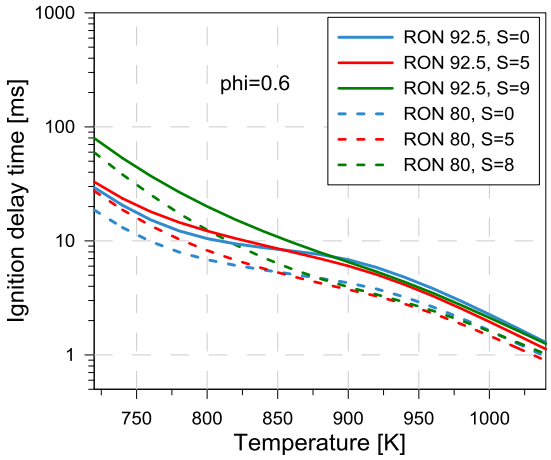

Figure 2. Ignition delay time results obtained through simulations for RON 92.5 (solid lines) and RON 80 (dashed lines) and the different sensitivities evaluated for a phi= 0.6 as function of the initial temperature in the reactor.

Figure 3 shows a global overview for a range of equivalence ratios from 0.5 to 1. This range of equivalence ratio was determined considering the LRF plus HRF injection at the condition of 50%@1800rpm, assuming a perfectly homogeneous mixture. It is clear that a stratification degree will be provided once the injection of the HRF is performed and this range can be extended, but again, the assumption is valid for comparison purposes for the different RONs and sensitivities. It should bear in mind that the HRF amount is just considered to determine the global equivalence ratio and it is not used in the simulations. Moreover, the early injections in the compression stroke should minimize the stratification effect. It is interesting to note that, again, the RON comparison has a major impact on the sensitivity. In Figure 3 (a), the ignition delay time is scaled according to the RON in a proportional manner. Nonetheless, once the toluene is introduced in the blends and the sensitivities values are increased (Figure 3 (b) and Figure 3 (c)) the proportional behavior is extinguished for lower equivalence ratios. Moreover, the more important differences in the reactivity between both RONs can be observed in the NTC affected zone, which is also shifted towards higher temperatures for the low RON evaluated.

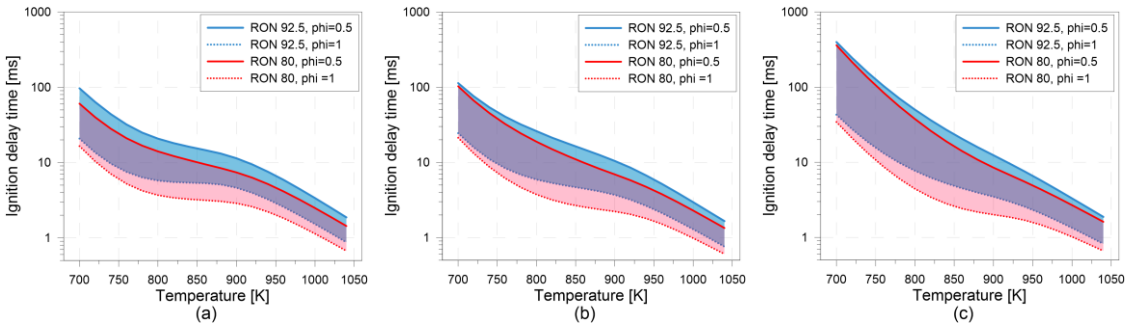

Figure 3. Ignition delay time range according to the proposed equivalence ratio limits based on the experiments (0.5 to 1) for the different RONs (92.5 and 80) and sensitivities obtained through simulations considering the same level of EGR dilution: (a) S=0, (b) S=5 and (c) S= max (9 for RON 92.5 and 8 for RON80).

3.1.2. Impact of fuel sensitivity on mixture reactivity for experimental conditions

As previously mentioned, the 0D evaluation of a dual-fuel combustion is a difficult task since it involves a degree of stratification that is not possible to represent in the simulations. Additionally, the HRF injections during the engine compression stroke represents a multiphase problem with the whole set of requirements to be solved. This restricts the correlations between the experimental and numerical results. In the light of this, during the experiments it was tried to obtain an operating condition with high GF to reach a combustion process near to a homogenous compression ignition, with low amount of diesel injected early in the compression stroke. This also helps to provide a more homogenous mixture. The condition that fulfilled these constraints was verified only at 1800 rpm and 50% of engine load, where the pressure and temperatures near to the combustion start are high enough to sustain an oxidation process of high GF levels without impacting the cyclic variability and combustion efficiency. The operating settings are presented at table 6 and the respective heat release rates (HRR) for the different RON and sensitivity values are presented in Figure 4. As it can be seen, the main difference in the calibration settings can be verified in the GF values. As the

reactivity increases for lower RONs, the pressure gradients exceed the mechanical constraints, requiring an increase of the HRF.

Table 6. Calibration settings obtained for each one of the RON for the different sensitivities at 50% of engine load and 1800 rpm.

RON	S	Speed	Load	P_{intake}	EGR	Soi_{Pilot}	Soi_{Main}	GF
92.5	[-]	[rpm]	[%]	bar	[%]	[CAD_{bTDC}]	[CAD_{bTDC}]	[%]
92.5	0	1800	50	2.11	47.62	60	50	78.81
92.5	5	1800	50	2.11	48.13	60	50	78.93
92.5	9	1800	50	2.1	47.85	60	50	79.05
80	0	1800	50	2.21	46.56	34	24	70.19
80	5	1800	50	2.22	47.09	34	24	70.92
80	8	1800	50	2.22	46.47	34	24	71.1

It is interesting to note that opposite behaviors are verified according to the RON used. In the case of RON 92.5, the modification of the sensitivity values results in a direct delay of the combustion process whilst at RON 80, no apparent modifications are perceived for the different set of sensitivities. To explain this behavior one can think that the temperature and pressures are different during the compression stroke for each condition. Nonetheless, Figure 5 shows no appreciable variations for these state properties during the compression stroke. Additionally, the dilution levels, intake temperature, air mass and equivalence ratio for each RON were maintained constant for the three experiments. It can be also verified from these profiles that the RON 80 has similar ignition time while the RON 92.5 does not present the same behavior.

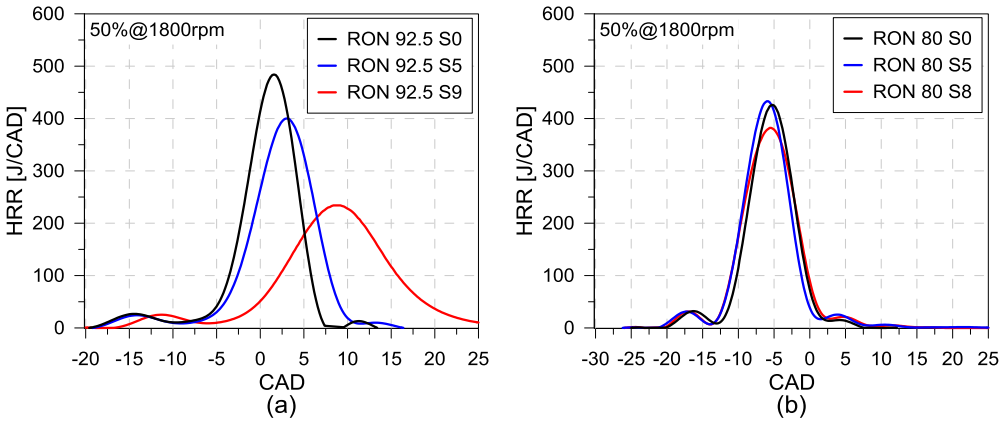

Figure 4. Experimental heat release profiles for the different RONs and sensitivities evaluated for the operating condition of 50%@1800rpm: (a) RON 92.5 and (b) RON 80.

As the pressure and temperature profiles were maintained for all the fuel blends, they were used as boundary conditions in the 0D analysis to evaluate the impact of the fuel sensitivity in the real conditions verified during the experiments. In this sense, a range from -60 to -5 CAD was chosen addressing the final of the compression stroke, where the corresponding values are marked by a symbol on the graphs. The equivalence ratio experimentally measured is the same for both fuels. Nonetheless, as a consequence of the required modifications of the PRF 80, a lower GF value was used during the experiments. Therefore, the initial vector of mass fraction components was recalculated to account for this modification. It is important to mention that each reactor is independent on the crank angle, where the conditions of the first reactor do not influence the second one.

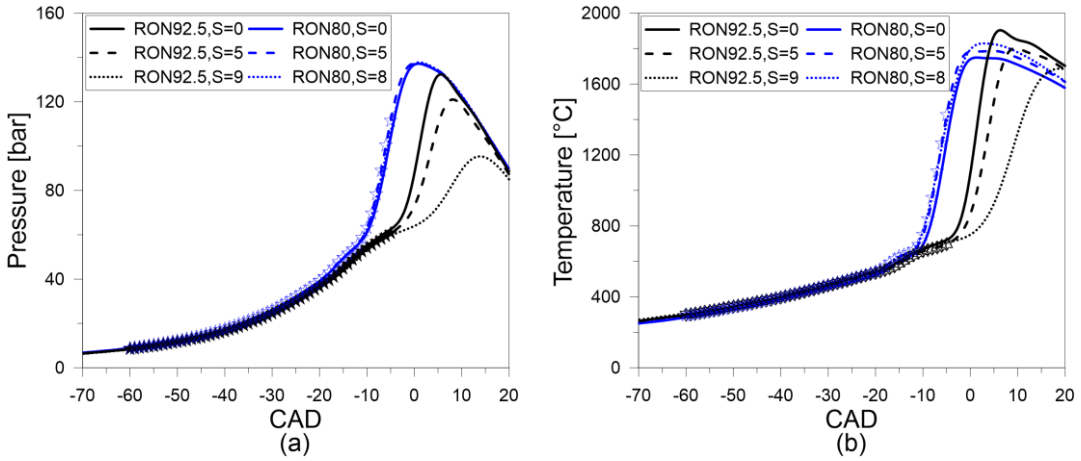

Figure 5. Experimental pressure profiles and calculated temperatures for the different RONs and sensitivities evaluated for the operating condition of 50%@1800rpm: (a) pressure and (b) temperature.

The results from the 0D model are presented in Figure 6. As it can be seen, the values of induction follow the same trend aforementioned. However, when the values are compared in terms of CAD, differences of almost 10 CAD can be found to have the same values of ignition delay time for both mixtures. This result agrees with those verified in the experimental HRR, demonstrating that the mixture reactivity is a dominant mechanism for the combustion start. It is also interesting to note that there is a correlation between the ignition delay times from the model and the LTHR onset in the experiments. In the case of RON 80, all the sensitivities present similar ignition delay times in the simulations for the CAD at where the LTHR is noticeable (≈-20 CAD). When this is contrasted with the experiments, it is possible to see that all the mixtures present the same experimental ignition delay. By contrast, having as reference the CAD where the low temperature heat release (LTHR) starts for the RON 92.5, it is possible to see that both S=0 and S=5 presents similar ignition delay times. Nonetheless, it is possible to verify that S=9 presents higher values, indicating a lower reactivity. The confrontation of the numerical and experimental results for this RON demonstrate the same trend, reinforcing that the sensitivity variation is a key factor during the first stage of the combustion development.

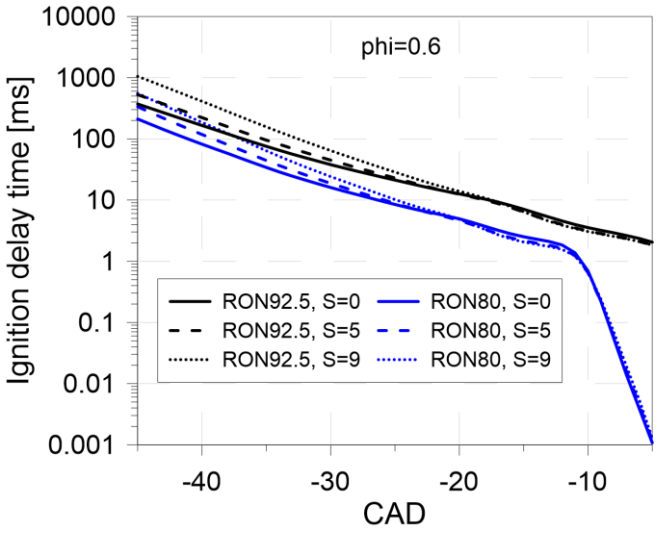

Figure 6. Simulated ignition delay times for the different temperature and pressure values verified during the compression stroke (45 up to 5 CAD bTDC) for both RONs and the different sensitivity evaluated.

Figure 7 shows the ignition delay time results for the same phi range than that evaluated in section 3.1.1 considering the different GF and EGR values from the experiments. It is important to bear in mind that even if a stratification field exists, all the sensitivities should present similar phi distribution, since the conditions where the HRF is injected are maintained as close as possible. From Figure 7, it is possible to verify that the deviations of the ignition delay times from S=0 to S=5 are more apparent for lower temperatures at the phi range evaluated, indicating the importance of the NTC behavior. As the sensitivity is extended to its maximum value, the differences become apparent and the deviation from the S=0 is evident. From the graph analysis, it is possible to infer that the RON 80 always present smaller ignition delay times than RON 92.5, considering a similar phi. It is also interesting to note, that the higher mixture reactivity provides a larger zone in conditions under a fixed values (e.g., 10 ms). In this sense, it should be expected lower deviations in the experimental ignition delay time once the conditions are inside this zone for RON 80.

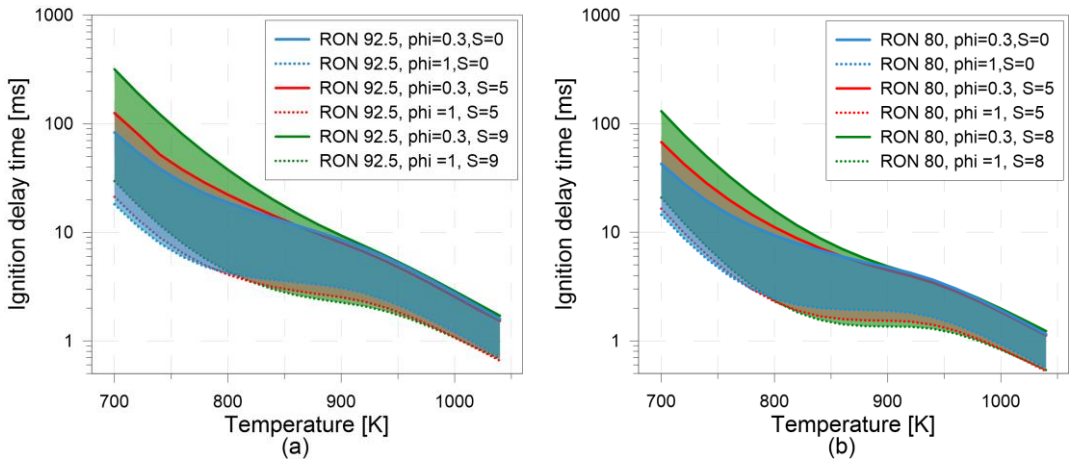

Figure 7. Ignition delay time range according to the proposed equivalence ratio limits based on the experiments (0.3 to 1) for the different RONs (92 and 80) and sensitivities obtained through simulations considering the differences of dilution and gasoline fraction of each one of the blends.

3.1.3. Experimental results for primary reference fuel 92.5

In addition to the previous results, extra operating conditions were evaluated to explore the effect of the sensitivity variation in a range of engine loads and speeds. The first fuel blend analyzed is a RON 92.5 with different sensitivity values (0, 5 and 9). As it will be demonstrated, the operating conditions in which the fuel is evaluated has major impact on the HRR, dictating the differences among the sensitivities. This relies on the fuel chemistry and state properties that can lead the operating condition to be found inside an NTC affected zone or not. Figure 8 presents two low load operating conditions at different engine speeds, where the diesel injection timings were fixed around 29 (pilot injection) and 19 (main injection) CAD bTDC. This means that, at the moment of the combustion start, the in-cylinder reactivity is a function of the diesel and gasoline quantity. Therefore, it is not possible to decouple the chemistry of these fuels. Moreover, the injections near to the combustion start means a high degree of mixture stratification as the mixing time is short since the difference between the start of the main injection and the LTHR (≈7 CAD).

As it can be seen in Figure 8, for both operating conditions, a similar trend is verified with early combustion start for S=0 and delayed combustion for S=9. It should be remembered that the injection strategy is the same for each one of the different sensitivities used. As previously demonstrated, such behavior can be found in zones near to the start of the NTC zone where the sensitivity lines of zero and five cross each other, presenting short ignition delay time for S=5. As the sensitivity is increased, the ignition delay time is prolonged, which can be an explanation from the different trends verified in these conditions.

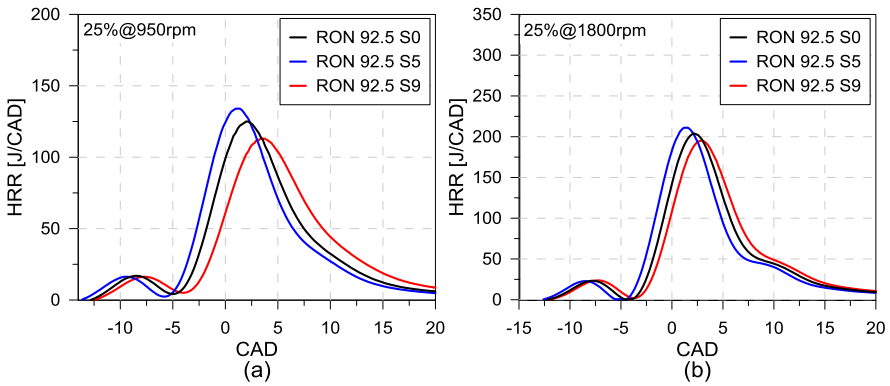

Figure 8. Experimental heat release profiles for the different RONs and sensitivities evaluated for the operating condition (a)25%@950rpm and (b) 25%@1800rpm.

At full load operation, for both 1800 and 2200 rpm, the effect of the sensitivity at the combustion start is minimized, since the temperature and pressure values where the combustion starts are higher enough to avoid the NTC zone, as it is demonstrated in Figure 9. It is also interesting to note that the variation of the sensitivity does not affect the low temperature heat release, also contributing to obtain combustion start for both operating condition whichever the sensitivity. Nonetheless, as the combustion proceeds, it can be seen a deviation from the mixture of S=9. This behavior is not fully understood, requiring additional evaluations by means of detailed chemical Kinect coupled with 3-D simulations to capture the phenomena that should be governing the

conditions at high temperature- high pressure. One possible assumption is that the high pressure found in these conditions (>140 bar) could be extinguishing the zone where NTC does not occur.

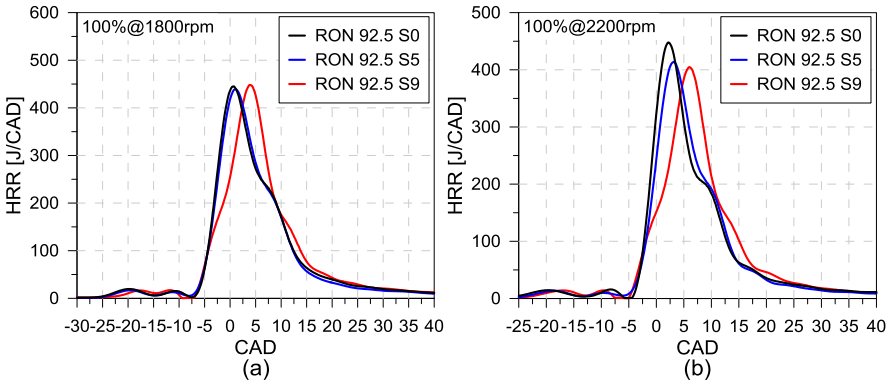

Figure 9. Experimental heat release profiles for the different RONs and sensitivities evaluated for the operating condition (a) 100%@1800rpm and (b) 100%@2200rpm.

3.1.4. Experimental results for primary reference fuel 80

A similar evaluation than that performed in the previous subsection was applied to the HRR profiles obtained for the PRF80. Figure 10 shows the results obtained for the operating conditions at 25% of engine load and 950 and 1800 rpm, respectively. At these conditions, small differences among the different heat release profiles for each one of the sensitivities evaluated is observed, independently on the operating conditions. One possible justification relies on the wider temperature range not affected by NTC that was previously presented. In this sense, the temperature/pressure path along the compression stroke and near to the combustion start avoids the NTC zone, resulting in similar reactivity for each one of the fuel blends. Consequently, the impact of the different sensitivities is reduced.

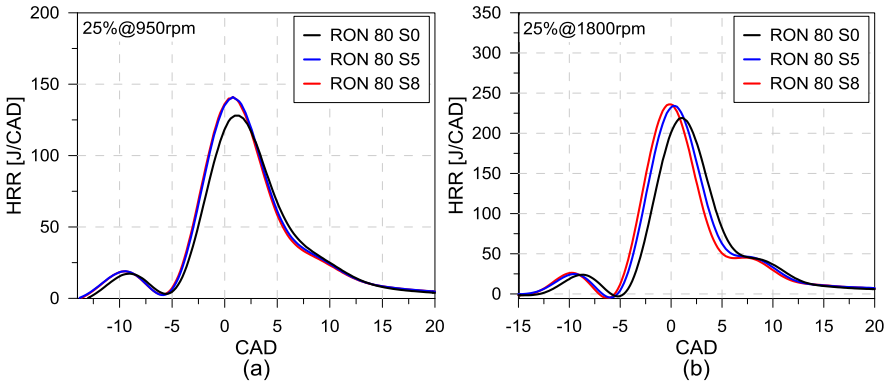

Figure 10. Experimental heat release profiles for the different RONs and sensitivities evaluated for the operating condition (a) 25%@950rpm and (b) 25%@1800rpm.

At full load conditions (Figure 11) it can be seen noticeable differences in the combustion start and development for the sensitivities evaluated. The first remarkable difference is related to the low temperature heat release. As the mixture reactivity is considerable higher, the quantity of heat released before the start of the main combustion process is more pronounced than the case of the RON 92.5. Therefore, the modifications of pressure and temperature attributed to this are enough to affect the ignition process. As this low temperature heat release occurs at low temperatures and pressures, it presents differences in its absolute value and phasing due to the differences in the sensitivity values. They are directly scaled with the trends verified to the NTC affected zone, demonstrating that the S=0 is the most reactivity blend while S=8 is the lowest one. This also affects the peak of heat release from the premixed part of the combustion. Once the combustion process is delayed towards the top dead center (TDC), the conditions at which the combustion starts have higher temperature and pressure values. Therefore, the combustion is accelerated, and the amount of energy released in the same period of time is higher, tailoring the heat release rate (HRR) shape. The final part of the combustion is controlled by the diesel injection, resulting in the similar end of combustion, independently on the sensitivity and operating condition evaluated.

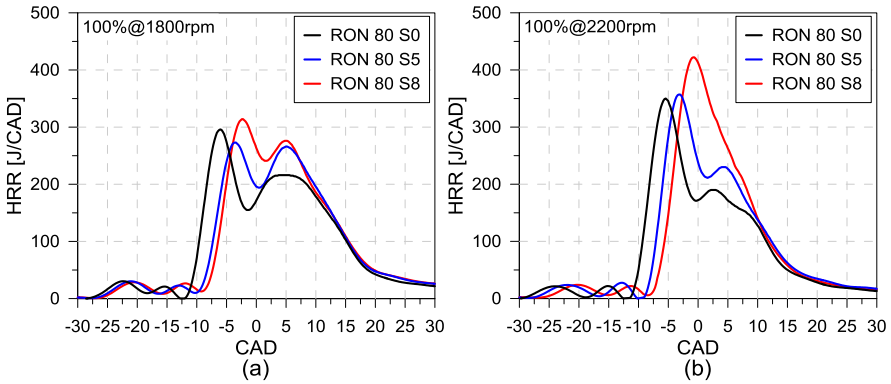

Figure 11. Experimental heat release profiles for the different RONs and sensitivities evaluated for the operating condition (a) 100%@1800rpm and (b) 100%@2200rpm.

3.2. Performance and emissions results

This section evaluates the fuel sensitivity effect on the performance and emissions from the dual-mode dual-fuel combustion. The first subsection is dedicated to the results with RON 92.5 and the second subsection shows the results found with RON 80.

3.2.1. Experimental results for research octane number 92.5

To evaluate the fuel sensitivity effect on the performance and emissions, the air management and injection settings were maintained as similar as possible for all the fuel blends at each operating condition tested. In that way, the differences on the average parameters can be directly attributed to the different sensitivity values. Three operating conditions were selected to study the different engine loads and speeds (25%@950rpm (fully premixed), 50%@1800rpm(fully premixed) and 100%@2200rpm (dual fuel diffusive)), and therefore different combustion strategies. Table 7 summarizes the main engine settings for the conditions tested.

Table 7. Engine settings and boundary conditions for the three points evaluated and the different sensitivities for RON 92.5.

S	Speed	Load	P_{intake}	T_{intake}	EGR	Soi_{Pilot}	Soi_{Main}	GF
[-]	[rpm]	[%]	bar	[^oC]	[%]	[CAD_{bTDC}]	[CAD_{bTDC}]	[%]
0	950	25	1.08	41.37	44.91	29	19	46.56
5	950	25	1.09	42.39	45.02	29	19	46.95
9	950	25	1.09	43.61	44.95	29	19	47.37
0	1800	50	2.11	65.19	47.62	60	50	78.81
5	1800	50	2.11	64.37	48.13	60	50	78.93
9	1800	50	2.10	63.20	47.85	60	50	79.05
0	2200	100	2.53	58.50	20.26	-	11	38.93
5	2200	100	2.54	58.38	20.16	-	11	38.89
9	2200	100	2.54	57.26	20.05	-	11	39.30

Figure 12 shows the impact of the fuel sensitivity variation on the fuel consumption for these conditions. As it can be seen, all the operating conditions do not follow the same trend. This can be attributed to having different gasoline fractions as well as in-cylinder temperature and pressure for each case. Moreover, each operating condition is representative of a different combustion strategy. For both 25%@950rpm and 50%@1800rpm, a fully premixed strategy with a GF higher than 50% is used. As a consequence, the sensitivity variation plays a fundamental role on the combustion development, resulting in a higher fuel consumption as the sensitivity increases. This can be attributed to the higher combustion durations discussed in section 3.1.2. In the case of 50%@1800rpm, the sensitivity effect is even more pronounced as the LRF represents more than 80% of the total provided energy. Therefore, as the sensitivity is increased, decreasing the reactivity of the fuels, the combustion process is longer, which impairs the fuel-to-work conversion efficiency. By contrast, at 100%@2200rpm, the GF values are decreased to avoid excessive pressure gradients. Additionally, the diesel injection strategy is modified towards a diffusive combustion. Therefore, the total energy provided by the LRF is low and the bulk part of the combustion process is

attributed to the diesel. Under these conditions, the effect of the sensitivity is overshadowed. Even though, some slight differences without a clear trend can be observed in the fuel consumption.

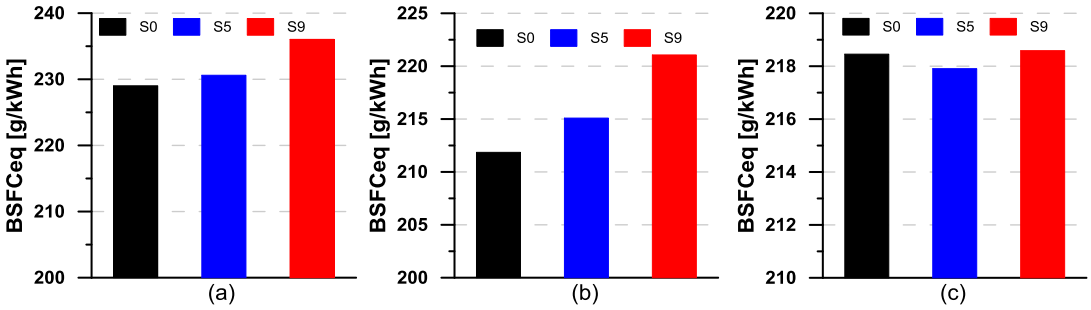

Figure 12. Equivalent brake specific fuel consumption for RON 92.5 with sensitivities of 0, 5 and 9 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

From the analysis of Figure 13 and Figure 14 t is also possible to verify that the sensitivity has an important role on the engine-out emissions. Figure 13 depicts the effect of the sensitivity on the NOx and soot emissions for the different operating conditions evaluated. For the first two operating conditions, the engine-out soot is virtually zero as a consequence of the high degree of premixing and only the NOx emissions can be analyzed. As it can be seen, the NOx levels follow the opposite trend to that verified for the BSFC at these conditions. This behavior is widely addressed in the literature [45]. At full load operation, the limits of both NOx and soot must be relaxed as it is required a dual-fuel diffusive combustion to avoid the high pressure gradients that should be found in the case of a premixed combustion. Despite of the differences in sensitivity, low variation was verified for both emissions in this condition. This is mainly attributed to the low GF levels that are used in this condition. In this sense, the combustion process is dominated by diffusion, where the different characteristics of the fuels have low impact on the HRR and final emissions

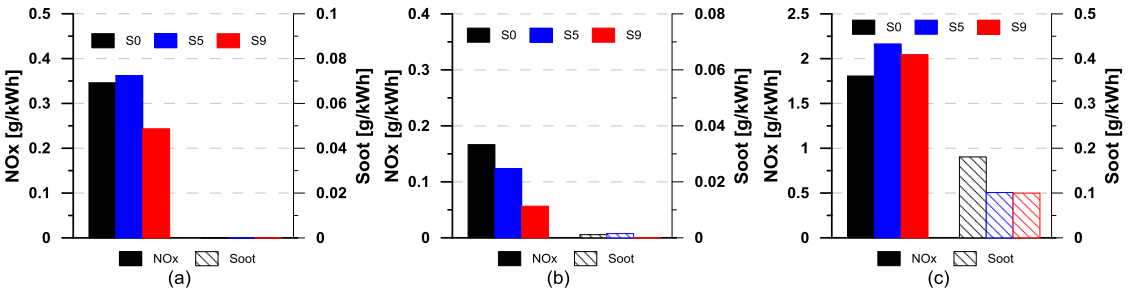

Figure 13. Nitrogen oxides and soot emissions for RON 92.5 with sensitivities of 0, 5 and 9 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

Figure 14 shows the unburned hydrocarbons and carbon monoxide emissions. As it can be seen, the major differences for the different sensitivities are presented in the operating condition at 50%@1800 rpm. The particularity of this condition is the use of a higher gasoline fractions. This is possible because the pressure and temperatures at the cycle start guarantee proper conditions to obtain a stable combustion process. Moreover, high EGR levels can be used to reduce the pressure gradients as the air loop system is not constrained. In this sense, variations on the LRF properties have a major impact on the combustion efficiency. This is directly correlated with the behavior verified in the HRR traces, leading to higher amounts of CO and HC as the sensitivity increases. Finally, in the full load condition, both emissions present low values and lower differences between the fuels as a consequence of the diffusive combustion, which governs the oxidation process and reduces the impact of the sensitivity.

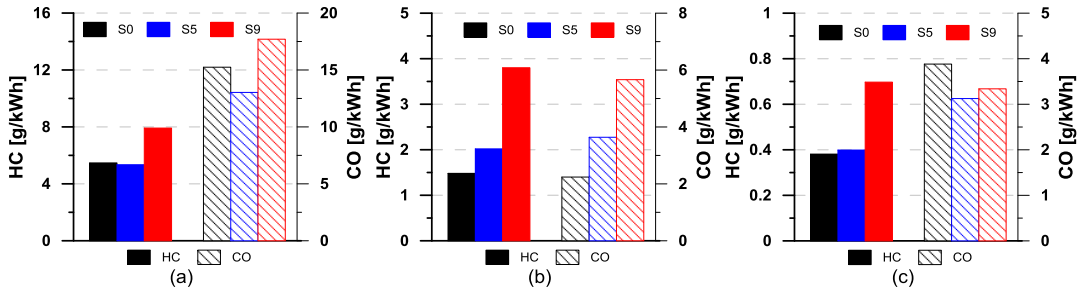

Figure 14. Unburned hydrocarbon and carbon monoxide emissions for RON 92.5 with sensitivities of 0, 5 and 9 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

3.2.2. Experimental results for research octane number 80

A similar analysis than that performed in the previous section was performed for the RON 80 fuel. For each operating condition, the three sensitivities were evaluated maintaining the boundary conditions as similar as possible among each other as presented in Table 8.

Table 8. Engine settings and boundary conditions for the three points evaluated and the different sensitivities for RON 80.

S	Speed	Load	P_{intake}	T_{intake}	EGR	Soi_{Pilot}	Soi_{Main}	GF
[-]	[rpm]	[%]	bar	[°C]	[%]	[CAD_{bTDC}]	[CAD_{bTDC}]	[%]
0	950	25	1.08	45.19	47.61	29	19	47.02
5	950	25	1.08	45.17	48.39	29	19	47.26
8	950	25	1.07	45.47	47.39	29	19	47.64
0	1800	50	2.21	78.11	46.56	34	24	70.19
5	1800	50	2.22	77.06	47.09	34	24	70.92
8	1800	50	2.22	76.01	46.47	34	24	71.10
0	2200	100	2.72	73.86	20.18	-	13	36.58
5	2200	100	2.74	73.18	20.67	-	13	36.86
8	2200	100	2.71	73.97	20.52	-	13	37.04

Figure 15 shows the results for the brake specific fuel consumption (BSFC). At low load conditions, the fuels with S=5 and S=8 have a slight increase of the BSFC values due to the early combustion start, releasing more energy during the compression stroke and then decreasing the cycle efficiency. As the load is increased, the differences become even lower. For the operating condition of 50%@1800 rpm, contrary to the RON 92.5, the BSFC is weakly impacted by the sensitivity. In this case, the small increase in the BSFC can be attributed to the increase in the combustion duration, as depicted in Figure 4. In the full load operation, the sensitivity increase results in lower fuel consumption. As the ignition delay time increases with the sensitivity for this condition, and the end of the combustion is defined by the diesel injection, the combustion duration is shortened

inside this crank angle range. Therefore, the heat transfer losses due to the combustion duration are decreased, improving the engine efficiency.

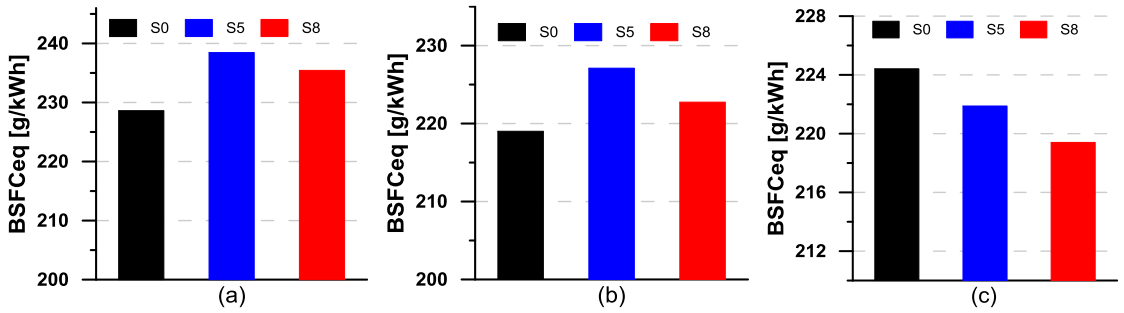

Figure 15. Equivalent brake specific fuel consumption for RON80 with sensitivities of 0, 5 and 8 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

Figure 16 shows the engine-out NOx and soot emissions for the three operating conditions evaluated and the different sensitivities. For the operating condition of 25%@950rpm, small differences in the NOx emissions are seen for the sensitivities evaluated. Recalling the results of the HRR analysis, this condition showed similar HRR profiles, indicating the low influence of the sensitivity on the combustion development. The soot emissions produced at low engine load are virtually zero as a result of the high degree of premixing. In this sense, no variation can be perceived. At full load operation, both NOx and soot demonstrated to be not affected by the different sensitivities evaluated despite of having different combustion developments. This can be attributed to the balance between the combustion duration and the HRR peak. The NOx production is a function of the maximum temperature and the residence time of the nitrogen (N_2) molecules inside this high temperature zone. When higher sensitivities are used, this effect should be balanced, since the cases where the maximum peak of HRR are verified are those where the combustion is the shortest.

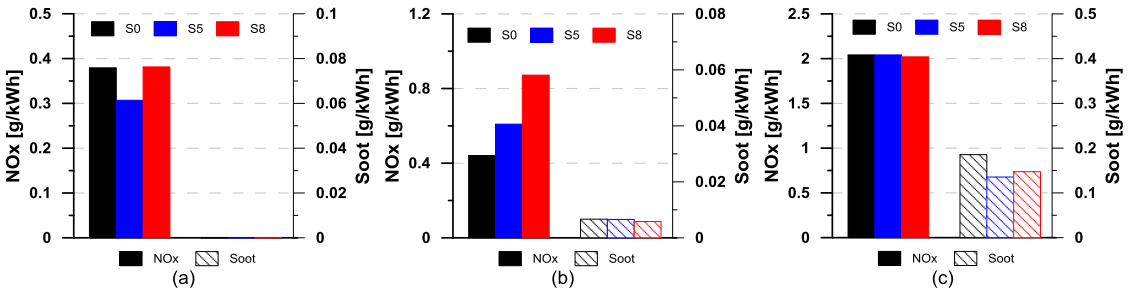

Figure 16. Nitrogen oxides and soot emissions for RON80 with sensitivities of 0, 5 and 8 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

Finally, the results of unburned hydrocarbons and carbon monoxide emissions for the RON 80 with different sensitivities are presented in Figure 17. The low dispersion in the values of both pollutants for 25%@950rpm must be explained by the small differences in the HHR. The main mechanisms that should be responsible of this behavior were previously discussed in section 3.1.4, being the higher reactivity of this fuel the most prominent one. The higher reactivity of the fuel also improves the combustion process reducing the total unburned hydrocarbons emitted, even in condition with high GF values as 50%@1800rpm (Figure 17 (c)). As it can be seen in Figure 17 (c), the results of unburned hydrocarbons for 100%@2200rpm are really low compared to the other operating conditions. Moreover, it can be noted that they are approximately half than those verified for RON 92.5. This can be related to the higher reactivity of the LRF and the lower GF values used for this point as a requirement to avoid the maximum pressure gradients.

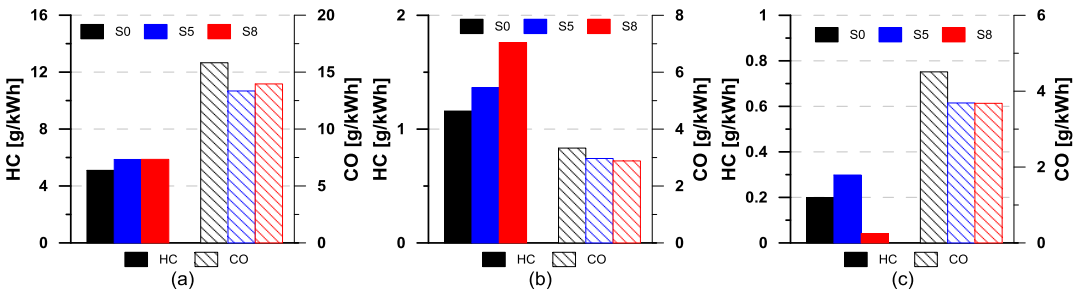

Figure 17. Unburned hydrocarbon and carbon monoxide emissions for RON80 with sensitivities of 0, 5 and 8 at (a) 25%@950, (b) 50%@1800, (c) 100%@2200.

4. Conclusions

This paper investigated the impact of the fuel sensitivity on the combustion process of a multi-cylinder engine operating in dual-mode dual-fuel combustion (diesel/gasoline) concept using low reactivity fuels with different octane numbers by means of 0-D numerical calculations as well as experimental evaluations. The numerical evaluation allowed to conclude that:

- Fuel sensitivity has a major impact on the ignition delay times being able to surpass the effect of the ON as the case of RON 92.5 S0 and RON80 S8.
- RON 80 provides a higher zone where the sensitivity does not affect the ignition delay time.
- RON 92.5 presents almost twice the ignition delay times than those verified for the RON80.

Besides, with the investigations on the multi cylinder engine platform, it was possible to verify the impact of the sensitivity on the different combustion regimes of the DMDF concept. The major conclusions are:

- RON 92.5 presented higher difference in the combustion start for low to medium load operating conditions. At high loads, the differences appeared during the combustion development.
- RON 80 had similar combustion delays at low load and at medium load conditions. As the engine load increases towards the full load operation, the high reactivity of this fuel affects the LTHR zone evolution. In this sense, high sensitivity values result in delayed combustion start. Nonetheless, as the end of combustion in

these conditions are defined by the diesel injection, this decreases the total combustion duration contributing to improve the final fuel consumption.

Based on this, it is possible to conclude that the LRF characteristics have a major impact on the dual-fuel combustion development in a wide range of engine load, speed, gasoline fraction, dilution levels and combustion regimes. Therefore, such characteristics must be considered in the determination of surrogates and during numerical combustion evaluations for this type of technology. The differences verified presents an additional degree of freedom in the problem that can seems complex to reproduce. This is also a critical point in advanced combustion modes, where the fuel composition has a major impact on the performance of the engine, requiring stricter fuel formulation to assure the same performance than those verified during the development phase. Moreover, understanding the impact of the fundamental fuel characteristics allows a proper fuel design that enables the use of such combustion modes in real applications. This can guarantee the success and allows to extract the benefits of these systems in the CO_2, NOx and soot reduction, allowing to simplify the aftertreatment system, reducing the final cost of the vehicle.

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Abbreviations

BSFC: Break Specific Fuel Consumption

bTDC: Before Top Dead Center

ATS: Aftertreatment System

CAD: Crank Angle Degree

CFD: Computational Fluid Dynamics

CFR: Cooperative Fuels Research

CO: Carbon Monoxide

CO_2: carbon dioxide

DI: Direct Injection

DMDF: Dual-mode Dual-fuel

EGR: Exhaust Gas Recirculation

ECU: Electronic Control Unit

FSN: Filter Smoke Number

GF: Gasoline Fraction

HC: Hydro Carbons

HO_2: Hydroperoxil

H_2O_2: Hydrogen Peroxide

HCCI: Homogeneous Charge Compression Ignition

HRR: Heat Release Rate

HRF: High Reactivity Fuel

ICE: Internal Combustion Engine

LLNL: Lawrence Livermore National Laboratory

LRF: Low Reactivity Fuel

LTC: Low Temperature Combustion

LTHR: Low Temperature Heat Release

MON: Motor Octane Number

N_2: Nitrogen

NOx: Nitrogen Oxides

NO: Nitric Oxide

NO_2: Nitrogen Dioxide

NTC: Negative Temperature Coefficient

O_2: Oxygen

PFI: Port Fuel Injection

PRF: Primary Reference Fuels

RCCI: Reactivity Controlled Compression Ignition

RON: Research Octane Number

TDC: Top Dead Center

S: Sensitivity