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Development of an empirical test method to quantify the ϕ-sensitivity of liquid fuels

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ABSTRACT

Several researchers are investigating strategies to lower the emissions and increase the efficiency of combustion engines to reduce the negative impact on the environment and the climate from transportation. The low-temperature combustion (LTC) concept is the basis for some of these high-efficiency, low-emission combustion technologies. To maximize the combustion controllability of engines based on the LTC concept, the combustion behavior of fuel both at different equivalence ratios (ϕ) and under ϕ sweeps must be understood and planned precisely. The ϕ-sensitivity of a fuel explains its behavior at different engine loads or stratification levels. In this study, a new test method for empirically evaluating ϕ-sensitivity using a Cooperative Fuel Research (CFR) engine is proposed and the validity of the method is investigated. A modified CFR engine for homogeneous-charge compression ignition (HCCI) combustion is used to investigate the compression ratio (CR) sensitivity of different toluene–ethanol reference fuels (TERFs) in a research octane number (RON) range of 63–105. This study suggests a method to quantify the ϕ-sensitivity of different fuels and blends by measuring the compression ratio required to keep the CA50 constant while varying ϕ. It shows that the fuel composition greatly affects the fuel ϕ-sensitivity even for different blends with the same RON. The results also indicate that the coexistence of ethanol and toluene in a blend can generate the highest ϕ-sensitivity of the blend compared to other blends with the same RON. Fuel composition has a strong effect on emissions. The simultaneous effect of fuel composition and ϕ variation on the emission and stability parameters is nonlinear.

1. Introduction

Nowadays, it is well known by scientists that greenhouse gasses, primarily CO_2, are the main contributors to global warming [1]. The United Nations Environment Programme explained in its 2020 and 2021 reports that even if the Paris Agreement countries follow current legislation, global temperature will exceed 3 °C by the end of the century [1,2]. The resulting impacts of this temperature rise on the ecosystem is speculated to be irreversible [1,3]. As a result of global awareness of environmental issues, many researchers are focusing on the environmental aspects of their various fields of study [4–9].

As one of the well-known consumers of fossil fuels, the transport sector is seeking different ways to reduce its production of greenhouse gasses. One of the fastest ways to reduce emissions is to improve combustion engines by increasing their efficiency (i.e., lowering their fuel consumption) and replacing fossil fuels with renewable substitutes. Many studies have been conducted on renewable substitutes to replace fossil fuels, and various aspects of renewable fuels have been investigated [8–13]. Research is ongoing to introduce fuels that can be used in conventional combustion engines without a significant need for modification [13–18]. Another solution available to combustion engine manufacturers is improving combustion engines by applying more efficient combustion strategies that result in lower emissions [8,19–21]. The low-temperature combustion (LTC) concept is the basis of most of these high-efficiency and low-emission combustion technologies, such as homogeneous-charge compression ignition (HCCI), partially premixed combustion (PPC), and premixed charge compression ignition (PCCI). All LTC schemes are very sensitive to fuel type and the fuel/air

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mixture chemistry [19,22–25]. Direct-injection compression ignition combustion (DICI) is controlled by the start of injection (SOI), while spark ignition (SI) combustion is controlled by the spark timing which is not applicable to the HCCI, PPC, and PCCI combustion strategies. SOI is not a combustion control factor for HCCI combustion, but PPC, and PCCI combustion are somewhat controlled by the SOI. HCCI, PPC, and PCCI combustion strategies are considered as LTC combustion concepts. Since LTC controllability has a high dependency on the fuel/air mixture chemistry, a better understanding of the combustion properties of different fuel/air mixtures would help increase LTC combustion controllability and thereby efficiency and emissions[26–28]. Combustion control when ignition delay times increase and there is no positive ignition system in use, is one of the major challenges in the commercialization of LTC engines (HCCI, PPC, and PCCI).In modern engines that use conventional SI and compression ignition (CI) combustion technologies, the incoming unburned gas is lower in temperature and higher in pressure than in older-generation engines. Similar to the older-generation engines the research octane number (RON) and motor octane number (MON) test methods are defined with the unburned gas inside the combustion chamber higher in temperature and lower in pressure compared to the modern engines [29]. For this reason, many researchers claim that RON and MON are not proper indicators of fuel behavior or antiknock quality in modern engines [30–32]. RON and MON also do not provide any information about the auto-ignition of fuel under different load conditions. Other indexes such as the toluene number [32], octane index [29,33,34], HCCI Fuel Index [35], and Lund-Chevron HCCI number [30] are more appropriate for modern engines and modern combustion concepts.

An important parameter for the combustion behavior of a mixture is the equivalence ratio (ϕ). Any changes in ϕ affect emissions, fuel efficiency, and combustion stability in all types of engines and affect knock in SI engines. To complicate matters further there are differences in in-cylinder local conditions versus global conditions. Engines with late direct injection will typically have large temporal differences between local ϕ and global ϕ, while premixed strategies with homogenous charge, less so. A better understanding of the combustion characteristics of fuel at different ϕ levels is needed to better control combustion phasing in LTC engines [36–38]. Knock, in SI engines, which is driven by auto-ignition of the end gas, limits engine efficiency and could damages the engine. A proper understanding of the heat release rate (HRR) and auto-ignition behavior of homogeneous mixtures of various fuels and blends with different ϕ levels is needed to avoid knock [39–41].

John Dec and Magnus Sjoberg have developed the concept of ϕ-sensitivity [36,42–46] in a ϕ range of 0.2–0.4 during more than 15 years of research. They conducted several experimental campaigns examining HCCI combustion using a gasoline direct-injection engine and kinetic simulation in their studies. The main objective of those studies was to design a strategy based on fuel stratification to control low-temperature gasoline combustion (LTGC) and to understand the low-temperature reactions (LTRs) that affect LTGC. This series of studies led to the introduction of the initial ϕ-sensitivity number in 2006 and the latest ϕ-sensitivity number in 2019, with the latter being based on the kinetics simulation using the chemical kinetics simulation software, ANSYS CHEMKIN-PRO (Eq. 1).

$$\text{Norm } \phi - \text{sensitivity} = -\frac{1}{\tau}\frac{d\tau}{d\phi} \tag{1}$$

where ϒ is the ITHR ignition delay which refers to the end of the ITHR stage [46].

Sjöberg et al. found that in HCCI combustion, a ϕ higher than 0.42 increases the maximum pressure rise rate (PRR_{max}) beyond an unacceptable level and that combustion of a leaner (<0.32) mixture leads to misfire and strongly affects cycle-to-cycle variation [42,43]. They used partial fuel stratification (PFS) and intake charge boosting to increase the HCCI engine load, based on the idea that PFS enables higher fueling by decreasing the HRR at higher engine loads and that such boosting will enhance the low-temperature heat release (LTHR) and intermediate-temperature heat release (ITHR) in HCCI combustion [37]. PFS and boosting increases the ϕ-sensitivity and therefore leads to more effective and pronounced fuel stratification [44,47]. Their results indicate that the PFS injection strategy reduces the HRR of high-reactive but not low-reactive fuels [44,48]. Their finding shows the important role of ITHR as a characteristic of fuels that are ϕ-sensitive for LTGC; they explain that the start of LTHR is not ϕ-sensitive, while the start of the main combustion is ϕ-sensitive [46]. Conducting a ϕ sweep with an engine at constant CR will result in an excessive pressure rise rate at higher ϕ levels and misfire at lower ϕ levels, but still without affecting the LTHR [44].

Many other researches have been conducted on HCCI combustion and the most common operating range for these studies is ϕ=[0.2, 0.4] [38,49–51]. Several researchers have found that at the lean part of this range the combustion instability and cycle to cycle variations due to the late combustion phasing and low fuel energy is increasing. For an intermediate mixture around ϕ=0.3 the cycle to cycle variation decreases and combustion would be more stable. By increasing ϕ closer to 0.4 the cycle to cycle variation increases again but this time due to the high HRR and fast combustion. Most of the HCCI researches show that for a stable HCCI combustion the ϕ must be maintained around 0.3. This doesn't means that there is no need to understand the processes at the rich HCCI limit; but explains the limitation and necessity of finding other methods to investigate the HCCI rich range [26,52,53].

To achieve constant combustion phasing (e.g., CA50) at different ϕ levels of one fuel, the intake temperature (T_{in}) or CR must be adjusted. In this study, a constant combustion phasing of CA50 (the crank angle degree at which 50% of total accumulated heat is released) has been achieved by adjusting the CR. A Cooperative Fuel Research (CFR) engine is well known for its variable compression ratio (CR). Pintor et al. explained that the ϕ-sensitivity depends on the CR of the engine, because the ϕ-sensitivity is controlled by the pressure/temperature trajectory prior to ignition [46]. Therefore a hypothesis of this study was that the adjusting of the CR to keep the CA50 constant will also keep the timing between the start of LTHR and the main combustion unchanged. This means that changing the CR for the purpose of constant combustion phasing at different ϕ levels will compensate for the effect of ϕ-sensitivity on ID. The reader should note that the definition of ID in different references is slightly different.

When the ϕ changes, some fuels or blends do not display great changes in the required pressure/CR for the start of ignition, so these fuels a have lower ϕ-sensitivity [44]. These fuels have lower COV_{IMEP} and PRR_{Max} during homogeneous SI at both low and high load if they have a high RON as well [46] and are also more resistant to knock. This is mainly because in case of any non-homogeneity in the combustion chamber, mixtures with different local ϕ levels behave very similarly in terms of ID and auto-ignition. These blends exhibit less LTHR and ITHR than do fuels with higher ϕ-sensitivity. On the other hand, fuels or blends that display high ϕ-sensitivity are more suitable for a stratified combustion, and would for example, be more suitable in LTGC if they are high-RON fuels; PPC if they are medium-RON; or in CI combustions if they are low-RON fuels [14,22,45,54–56]. Different fuels exhibit different pressure and temperature sensitivities to ϕ variation, and the ϕ-sensitivity is independent of RON and MON [46,57]. Therefore, a better understanding of fuel ϕ-sensitivity would facilitate the design of load-adaptive fuels that can tolerate different loads with minor combustion instability for different combustion concepts.

The objective of this study is to develop a test method for evaluation and quantification of liquid fuel ϕ-sensitivity, based on the fuel CR-sensitivity at a constant combustion phasing.

2. Test methodology

In this study a Cooperative Fuel Research F1/F2 (CFR-F1/F2) engine

Table 1
CFR-f1 engine specifications.

CFR engine	
Displacement volume	612 cm^3
Number of cylinders	1
Bore	83 mm
Stroke	114 mm
CR	Variable (4:1 to 18:1)
Number of valves	2
Intake valve opens	10° ATDC ± 2.5°
Intake valve closes	146° BTDC ± 2.5°
Exhaust valve opens	140° ATDC ± 2.5°
Exhaust valve closes	15° ATDC ± 2.5°

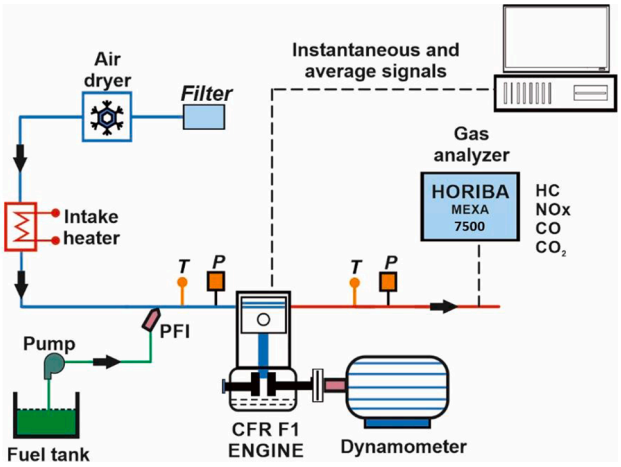

Fig. 1. Schematic of the modified CFR F1/F2 engine, PFI (port Fuel Injector), P (pressure sensor) and T (temperature sensor).

Table 2
Engine operating conditions.

Input parameters	Value	Variation
Intake charge temperature, T_{in}	323,373, 423 K	± 1 K
P_{in}	0.98 bar	± 0.03 bar
RPM	900	± 2
Coolant temperature	373 K	± 1 K
Oil temperature	330 K	± 8.5 K
CA50	3 °CA	± 0.5 °CA
CR	Variable	–
ϕ	0.31, 0.33, 0.35, 0.37	± 0.005

with variable CR is the experimental apparatus. A CFR engine is a standard engine designed to be used in developing a gasoline knock-test method. It is versatile as it can be used with fuels having different physical and chemical properties [58–61]. The engine specifications are presented in Table 1.

The CFR engine used in this study was modified for HCCI combustion and equipped with port fuel injectors, which, together with the intake air heater, allows a homogeneous charge at an adjustable temperature. Fig. 1 shows a schematic of the experimental apparatus. The time-averaged inlet charge temperature is measured by a thermocouple mounted in the intake manifold and close to the inlet valve. The time-averaged pressures were measured at the both intake and exhaust manifold with piezo resistive Kistler 4045A sensors. The In-cylinder pressure was acquired using a Kistler 6125C pressure transduce. The CFR engine is equipped with a rotary encoder with a 0.2 CAD resolution. In this study, 300 successive combustion cycles as well as 100 successive motored cycles are sampled for each operating point. The heat release is calculated from the pressure trace and the Woschni heat transfer model is used according to Heywood [62]. It has been assumed that the in-cylinder gas temperature, when the inlet valve closes (T_{IVC}) is known. T_{IVC} is calculated based on the measured intake temperature considering the effect of residual gas and the heat transfer to the wall. The heat release calculations are performed for each individual cycle and the presented figures in this paper are based on the mean value of 300 cycles. The error bars are based on standard deviation from the mean value. More details about heat release calculation can be found in [63]. The sampled motored cycles are used to the tune the heat release as close to zero as possible for the motored pressure trace. The in-cylinder pressure measurements are filtered and ensemble-averaged for every test point. An intake-air refrigerator unit is used to ensure constant intake-air humidity. The engine works in a naturally aspirated condition.

The engine cooling system provides a water temperature of 373 K. A Horiba Mexa 7500 analyzer system measures the NOx, HC, CO, and CO2. Oxygen and equivalence ratios (ϕ) are calculated from the measured exhaust gas emissions. In this study equivalence ratio is calculated based on the relative air–fuel ratio (λ). The lambda is calculated from the exhaust gas emissions, and for redundancy measured using etas sensor; then lambda is converted to the equivalence ratio as $\phi=\frac{1}{\lambda}$. The accuracy of measured/calculated λ using this setup is ± 0.02. Lambda adjustment with such accuracy is perfectly possible with the experimental apparatus of this experiment, and improve the accuracy of reported ϕ in the narrow range of this study. It was impossible to randomize all of the operating points, but from each RON group one fuel was selected and all of the operating points for that fuel were replicated three times randomly to check if the null hypothesis of this study holds. The null hypothesis is that performing the experiments on different days should not have statistically significant effect on the result parameters. This is done to make sure that the differences in required CR to keep the combustion phasing constant are not due to any error. In this study, the HCCI combustion has been performed at four ϕ levels, constant RPM, and three Tin values. The details of the experimental setup are presented in Table 2.

Combustion phasing was adjusted to a crank angle position of CA50 ≈ 3 °ATDC, this combustion phasing was achieved by adjusting the CR. The objective of keeping the CA50 constant using variable CR was to keep the ID constant at different ϕ levels (for more explanation, see "Results and discussion"). CA50 is the engine crank angle at which 50% of the total accumulated heat is released. According to Pintor et. al, pressure and oxygen have opposite effects on the ϕ-sensitivity property of a fuel [46]. A series of experiments demonstrated that increasing the equivalence ratio by throttling the engine decreases the intake pressure and at the same time increases the required CR to keep the CA50 constant. This would also mean that for leaner equivalence ratio boosting is necessary; throttling was also changing the P/T trajectory and the proportion of residual gas to the unburned gas and therefore changing the specific heat ratio and as a result would convolute the data analysis by increasing the number of variables. Therefore, in this study the ϕ was increased by increasing the fuel mass.

2.1. Fuel selection

Gasoline contains hundreds of different hydrocarbons, which makes it a complex mixture and less relevant as a reference fuel. In addition, gasoline is not a single homogenous product, but rather a collective name for several types of gasoline that varies in octane rating, heat of vaporization and other properties, depending on their intended application (road transport, handheld equipment, aviation) and local conditions (climate, altitude, emissions regulations). On octane rating alone, gasoline ranges from below 70 for straight-run gasoline (often referred to as naphtha) to above 100 for aviation gasoline. Both extremes are interesting. Naphtha-based gasoline is more efficient to produce than refined higher octane gasoline and has also shown promising results in advanced engine concepts [64–66], while high octane-rated gasoline

Table 3
Properties of fuel blend components.

Hydrocarbon class		Fuel	Molecular formula	RON	S = RON - MON	Boiling point, °C	Heat of vaporization, KJ/Kg	Calorific value, MJ/ Kg	Oxygen content, %
1	Oxygenated	Ethanol	C_2H_5OH	108	18	79	846	27	35
2	Aromatics	Toluene	$C_6H_5CH_3$	121	11	110	351	40.58	0
3	Iso-paraffins	Iso-octane	C_8H_{18}	100	0	99	305	44.46	0
4	n-paraffins	n-heptane	C_7H_{16}	0	0	98.5	321	44.56	0

Table 4
The fuel matrix.

Fuel		n-heptane, vol.%	Ethanol, vol.%	Toluene, vol.%	Calculated RON*	Calculated MON*	Measured RON	Measured MON	S*	S[1]	HoVJ/ g	$IMEP_{g,}$ bar
1	$T_{20}E_{40}RFn_{10}$	10	40	20	108.3	95.0	105.5[4]	91.1[4]	13.2	14.4[4]	536	3.0 — 4.5
2	$E_{50}RFn_{12}$	12	50	0	108.8	96.7	105.3[4]	91.3[4]	12.1	14[4]	591	3.2 – 4.4
3	$T_{25}E_{30}RFn_{40}$	40	30	25	84.52	77.2	85.4[4]	77.6[4]	6.9	7.8[4]	490	3.1 — 4.5
4	$E_{38}RFn_{43}$	43	38	0	84.4	78.9	84.4[3]	78.7[3]	5.4	5.7[3]	532	3.1 — 4.1
5	$T_{50}RFn_{30}$	30	0	50	82.7	74.1	83.8[2]	76.6[2]	8.5	7.6[2]	334	3.1 – 4.5
6	PRF84	16	0	0	–	–	84	84	–	0	307	3.0 — 4.3
7	$T_{10}E_{10}RFn_{49}$	49	10	10	63.0	59.1	63.1[4]	58.0[4]	4.0	5.1[4]	376	3.1 – 4.6
8	$E_{20}RFn_{55}$	55	20	0	63.7	59.6	63.2[4]	58.3[4]	4.2	4.9	432	3.2 – 4.5
9	$T_{40}RFn48$	48	0	40	63.3	56.3	63.7[2]	58.0[2]	6.9	5.7	332.9	3.1 – 4.6
10	PRF63	37	0	0	–	–	63	63	–	0	310	3.1 – 4.4

*Calculated based on a model introduced by Solaka Aronsson et al. [75].
[1] Based on measured RON and MON values from different references.
[2] From Kalghatgi et al. (2015) [68].
[3] From Solaka Aronsson et al. (2014) [75].
[4] Measured by project partner Saybolt AB Sweden.

allows more efficient SI-engines due to the reduced risk for pre-ignition and knock [24,41,67]. To avoid the issues with fluctuating properties, selecting a suitable surrogate fuel instead of using gasoline is an important aspect that helps limit the chemical and physical complexity of fuel testing and also establishes a baseline for further experiments on renewable fuels [32,68,69]. Various surrogate fuels are widely used in research; these fuels are categorized as single-component fuels, binary blends, and multi-component blends [55,70]. Primary reference fuels (PRFs) are blends of two paraffins, *iso*-octane and n-heptane. These were used to develop RON and MON test methods. PRFs have essentially zero octane sensitivity (S), meaning that the RON and the MON values for these blends are equal. However, for all types of gasoline and various alcohols, the S is above zero (RON > MON). Thus to design a test method that also accounts for fuel sensitivity S and is relevant for gasoline and future renewable fuels, surrogate fuels with a relevant range of S is required. Fuel sensitivity is important since with higher S, and not only higher RON, a higher knock resistance and ultimately higher efficiency can be reached [32,71]. Toluene reference fuels (TRFs) are blends of toluene and n-heptane and/or *iso*-octane. The S of TRFs is a positive number similar to that of gasoline. Aromatics are known to be responsible for S in the complex mixture that is gasoline. Toluene is the most important aromatic component of gasoline, in which its content can reach 35% [24,55,72]. The other components of surrogate fuels are oxygenated. Ethanol is widely used as a gasoline additive to enhance the octane number and also as a renewable fraction [70,73,74]. Therefore, for this investigation toluene–ethanol reference fuels (TERFs; containing toluene, ethanol, *iso*-octane, and n-heptane), which are oxygenated reference fuels, are selected. Since the aim of this study was to develop an empirical ϕ-sensitivity test method, different TERFs have been designed to cover a wide range of RON and MON values, from straight-run naphtha gasoline to neat ethanol, to ensure that the extremes are considered. The properties of the fuel blend components are presented in Table 3. Data is extracted from [24].

Toluene is responsible for the S in non-oxygenated surrogate gasoline. Ethanol is the oxygenated component that has high S and high RON. Iso-octane and n-heptane are two paraffins in the blends. Three groups of fuel were designed for this study. To separate the effect of fuel composition and octane number on the ϕ-sensitivity, a blending strategy was used where four different fuel compositions, TERF, TRF, ERF and PRF were blended to three different levels of RON with as similarly grouped MONs as possible. An in-house regression model provided by Solaka Aronsson et al. [75] was used to estimate the desirable volume of each component, while the blends RON and MON were measured by Saybolt AB Sweden. The measurements show that the model high RON of 108 is slightly over-predicted and in reality, around 105. The detailed information is presented in Table 4, where the HoV is calculated using a mass based linear correlation. An example of the naming convention, $T_{20}E_{40}RFn_{10}$ is a blend consisting of 20% toluene, 40% ethanol, and 10% n-heptane. The *iso*-octane is used as a filler, so in this case the blend is 30% *iso*-octane. All the blending ratios are volumetric ratios.

2.2. Definition of CAD selection for the start of LTHR and main combustion

There are different criteria and definitions for the start of combustion and the auto-ignition point of fuels in a CI engine [20,30,76,77]. Some studies select the crank angle at which a certain percentage of accumulated heat is released [61]. This method is valid when the total accumulated heat release (TAcHR) is almost constant at different operating points for one fuel, basically at a constant load. Because this method is relative to the quantity of TAcHR, when the TAcHR is high, the percentage-wise selected point will move closer to the top dead center (TDC), and when the TAcHR is low, this point will move away from the TDC. To exclude the effect of TAcHR on the selection of auto-ignition point, in some studies an absolute value of the HRR is selected as the auto-ignition point or the start of the main combustion [30,65,77]. In this study, the crank angle degree (CAD) at which the rate of heat release reaches 0.2 J/CAD is selected as the auto-ignition point or the start of combustion and early reactions [65,72]. The start of the main combustion or the high-temperature heat release (HTHR) is selected as the crank angle degree at which the rate of heat release reaches 5 J/CAD. This method for defining the start of the main combustion was recently used in a study of a CFR engine to define the detection of LTHR [77]. A combustion event without any clear heat release rate peak before the

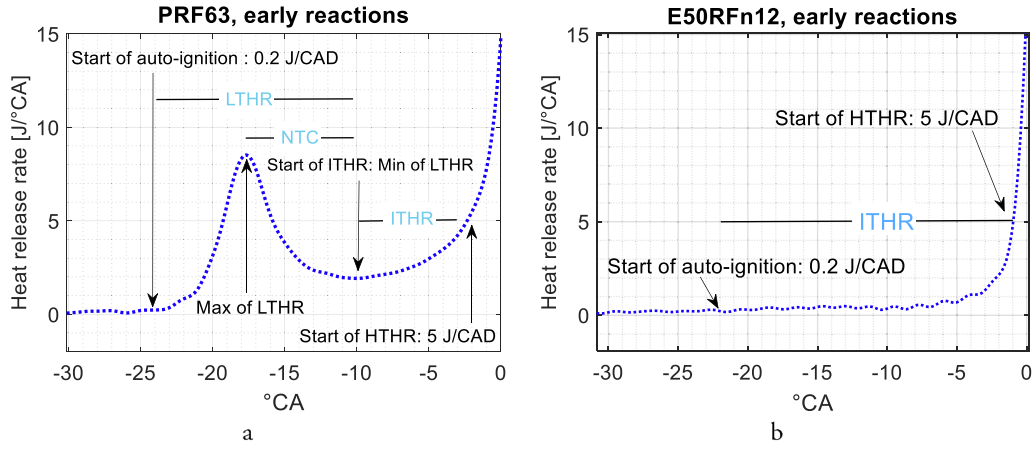

Fig. 2. CAD selection for start of LTR and HTR: a) HRR during the early reactions for two-stage combustion; b) HRR during the early reactions for single-stage combustion.

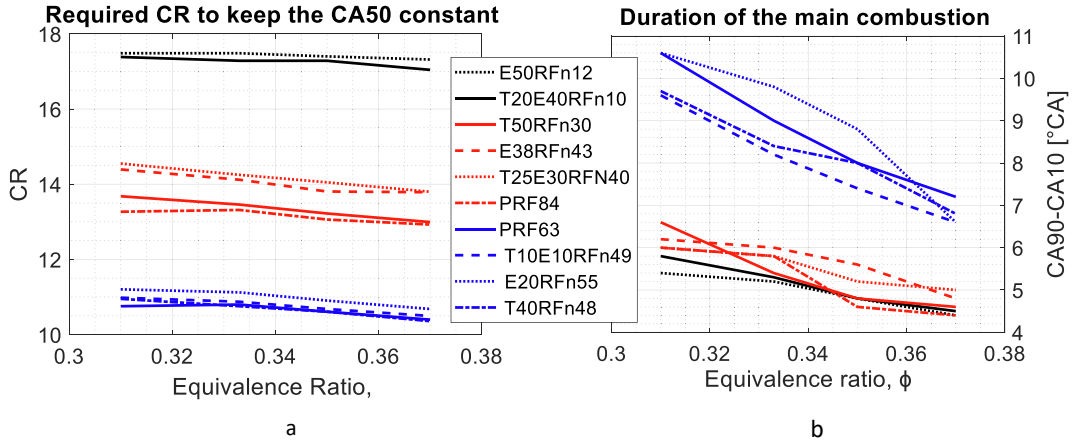

Fig. 3. Required CR to keep the CA50 constant (left) and main combustions duration (right) at different ϕ for all of the blends.

main combustion is defined as a single-stage combustion. For a single-stage combustion the early reactions period between 0.2 J/CAD to 5 J/CAD heat release rate is in this work defined as the ITHR. In this study the ID is defined as the timing between the start of auto-ignition and the start of the main combustion. For two-stage combustion the continuation of early reactions after the minimum of LTHR (Fig. 2) is considered as the ITHR [30,72,78]. The kinetic studies suggest that the early reactions before the start of the main exothermic reactions of the main combustion are responsible for ITHR; the main exothermic reactions are $H_2O_2 + M = OH + OH + M$, which M is called the third body and could be any molecule in the mixture [40,61,78–80]. Those early ITHR reactions are also terminating the exothermic LTHR reactions of alkyl radicals (R) and (H_2O) with O_2 [23,56,80]. Fig. 2 depicts different phases of early reactions for both two-stage and single-stage combustion. It also illustrates how different points are selected for the start of combustion, start of HTHR, etc.

3. Results and discussion

This section explains the dependency of ΔCR on the fuel ϕ-sensitivity. Different parameters and their dependency on the simultaneous variation in ϕ and CR are evaluated. Since the effect of ϕ-sensitivity is more significant at lower intake temperatures [45,46], the results at T_{in} = 323 K are selected for the method development and the main part of this discussion.

3.1. Variation in required CR for constant CA50 as an indicator of ϕ-sensitivity

In an engine with a constant CR, any increase or decrease in ϕ at constant T_{in} will shorten or lengthen the ID, respectively [42,46]. The variable CR of the CFR engine enables the adjustment and maintaining of constant combustion phasing (e.g., CA50) while varying the ϕ. Adjusting the CR to achieve a constant combustion phasing of CA50 ≈ 3° ATDC compensates for the effect of changing ϕ on the ID. This is due to the compensating effects of variation in ϕ and CR on the in-cylinder pressure, temperature, mass, and volume as well as the internal residual gas amount. Variation in these parameters will affect the early reactions and the auto-ignition of fuels but maintains the ID at a constant value. However, the duration of the main combustion is strongly affected by the ϕ variation, and a decrease in CR will not compensate for the effect of an increase in ϕ. This means that the lower in-cylinder pressure that is the consequence of a lower CR for a higher ϕ will compensates for the effect of ϕ variation on the ID but not on the main combustion duration. Fig. 3a shows the variation in CR required to keep the CA50 constant for the blends studied at T_{in} = 323 K. As can be observed, by increasing ϕ, the required CR decreases to keep the CA50 constant. Fig. 3b shows the durations of the main combustion for the different blends.

Despite the ϕ variation, the duration of early reactions (i.e., ID) stays constant for each fuel. This is mainly due to the reduction in the CR to

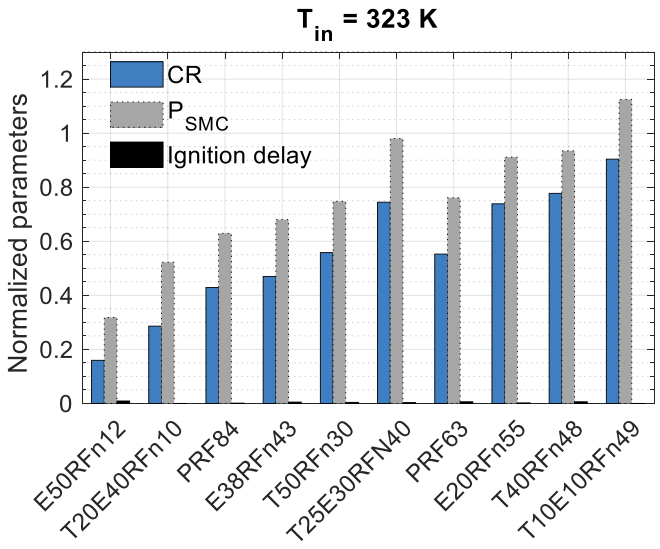

Fig. 4. Normalized parameters.

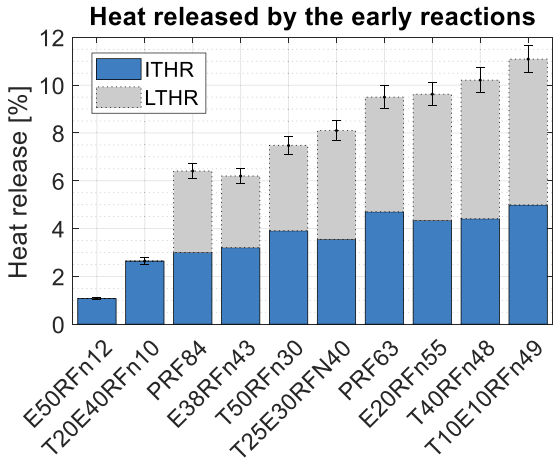

Fig. 5. Fraction of heat released during the early reactions. The error bars are the sum of the error of the LTHR and the ITHR.

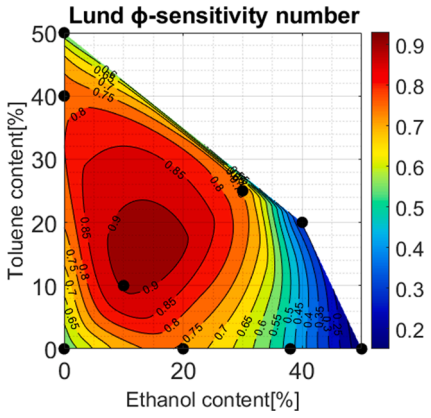

Fig. 6. Lund ϕ-sensitivity number as a function of ethanol and toluene.

maintain a constant CA50 at a higher ϕ. This CR reduction will reduce the in-cylinder pressure and prevent the shortening of the ID and early reactions due to the increased ϕ, which is expected in constant CR conditions [44].

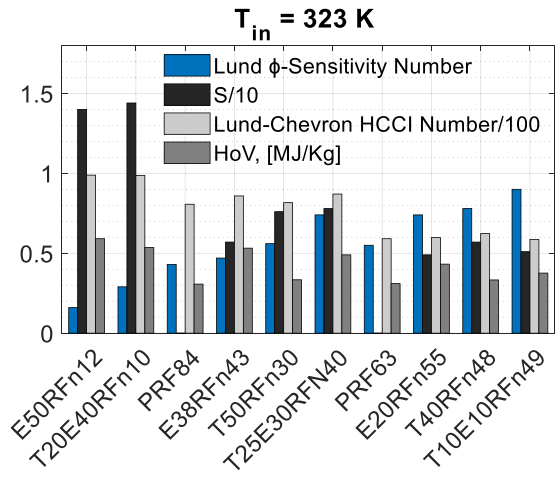

Fig. 7. Comparison of different fuel indexes with Lund ϕ-sensitivity number.

Fig. 4 shows normalized variation of CR; normalized pressure variation at the start of the main combustion (P_{SMC}); and normalized variation of ignition delay. Each normalized parameter is calculated based on the two operating points of each fuel blend with the highest and the lowest ϕ. The reader should note that decreasing the ϕ will require a higher CR to keep the combustion phasing (e.g., CA50) constant. The normalized CR (Norm CR) is calculated as follow: the CR for the operating point with the lowest ϕ, minus the CR for the operating point with the highest ϕ, divided by the CR for the operating point with the lowest ϕ and finally divided by the Δϕ (Eqs. 3–5). In this study, the Norm CR is selected as the ϕ-sensitivity number of the different blends.

$$\text{Norm CR} = -\frac{1}{\text{CR}}\frac{\Delta \text{CR}}{\Delta \phi} \tag{3}$$

$$\text{Norm P}_{\text{SMC}} = -\frac{1}{\text{P}_{\text{SMC}}}\frac{\Delta \text{P}_{\text{SMC}}}{\Delta \phi} \tag{4}$$

$$\text{Norm ignition delay} = -\frac{1}{\tau}\frac{\Delta \tau}{\Delta \phi} \tag{5}$$

The bar chart in Fig. 4 clearly shows that adjusting the CR to keep the CA50 constant can compensates for the effect of ϕ variation on the ID (indicated by the black bars, which are almost zero).

It can also be observed from this bar chart that the pressure variation at the start of the main combustion (P_{SMC}) follows the same trend as does the variation in CR required to keep the CA50 constant.

Fig. 5 shows the LTHR and ITHR as percentages of the TAcHR for each blend. The trend of different released heat during the early reactions following the trend of normalized P_{SMC} and CR between the different groups. In the same group, the PRF displays the highest average released heat during the early reactions. All other blends all contain ethanol and toluene, which both have quenching effects on the early reactions by scavenging the OH radical [81]. Considering the 3–5% variation between different blends, even this property follows the trend of normalized P_{SMC} and CR. It can be observed that the coexistence of aromatic and oxygenated hydrocarbons will increase the Norm CR (Eq. 3) and the released heat ratio during the early reactions (Figs. 4 and 5).

As explained in the "Test methodology" section of this paper, the variable CR of a CFR engine is the most distinctive feature of the engine. In the standard test method for RON and MON measurement the engine output is the digital counter reading (DCR), which is measured at each PRF level under defined and controlled conditions [58]. At first glance, the DCR does not give the reader (if not the operator of a CFR engine) any information about the thermodynamic conditions of the combustion chamber. In fact, the CR presented in this study is a thermodynamic translation of the DCR intended to be understandable for the vast

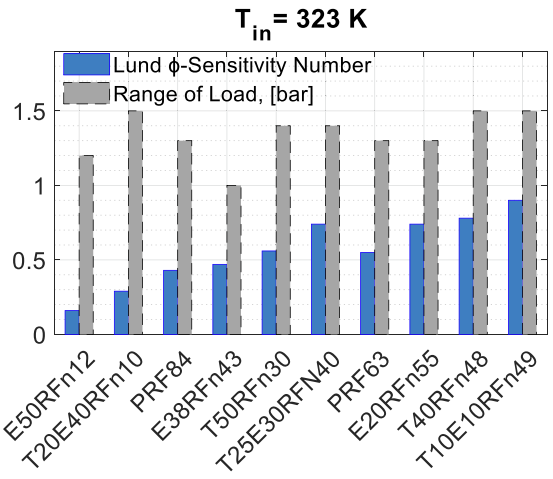

Fig. 8. Comparison of different fuel indexes with Lund ϕ-sensitivity number.

majority of researchers who are not directly studying a CFR engine. Therefore, in this study, the CR, not the DCR, has been introduced as the main output of the CFR engine. Moreover, the Norm CR (Eq. 3), which is an indicator of fuel response to ϕ variation during HCCI combustion, is defined as the Lund ϕ-sensitivity number. Fig. 6 is a visual summary of the effect of the volumetric percentages of ethanol and toluene on the of Lund ϕ-sensitivity number.

This plot clearly shows that a combination of aromatic and oxygenated hydrocarbons increases the Lund ϕ-sensitivity number more effectively. It can be concluded from this graph that ethanol and toluene have a combined effect on the Lund ϕ-sensitivity number except at oxygen contents above 10 V/V% (30 V/V% ethanol) in the blend. At higher concentrations of oxygen in the blend (i.e., above 10 V/V%), the effect of the oxygenated hydrocarbon is dominant.

Fig.7. is visualizing different fuel indexes for the blends of this experiment. Lund-chevron HCCI number, and S are divided to 100 and 10 respectively to make the bars more comparable visually, and HoV is reported in MJ/Kg. As Fig. 7. shows, there is no correlation between Lund ϕ-sensitivity number and Lund-chevron HCCI number. It is the same for HoV and S. Fig. 7. Depicts that there is no strong link or linear correlation between HoV and S, with the Lund ϕ-sensitivity number. Although the presented indexes in this bar chart are not linearly correlated, they can be a guide for fuel selection depending on a favorable combustion strategy.

As it is mentioned in the introduction, an important parameter to understand fuel load adaptability is the study of the ϕ-sensitivity behavior of different blends and fuels. This study suggests that there is a correlation between load adaptability of the tested blends and Lund ϕ-sensitivity number. As Fig. 8. displays, the evaluated ERFs in this study have lower Lund ϕ-sensitivity number and lower load adaptability compared to the TERFs or TRFs of the same group.

Generally both Lund ϕ-sensitivity number and load range are higher for the blends with aromatic content. This finding it's mainly due to the higher accumulated heat that TERfs and TRFs are releasing during the

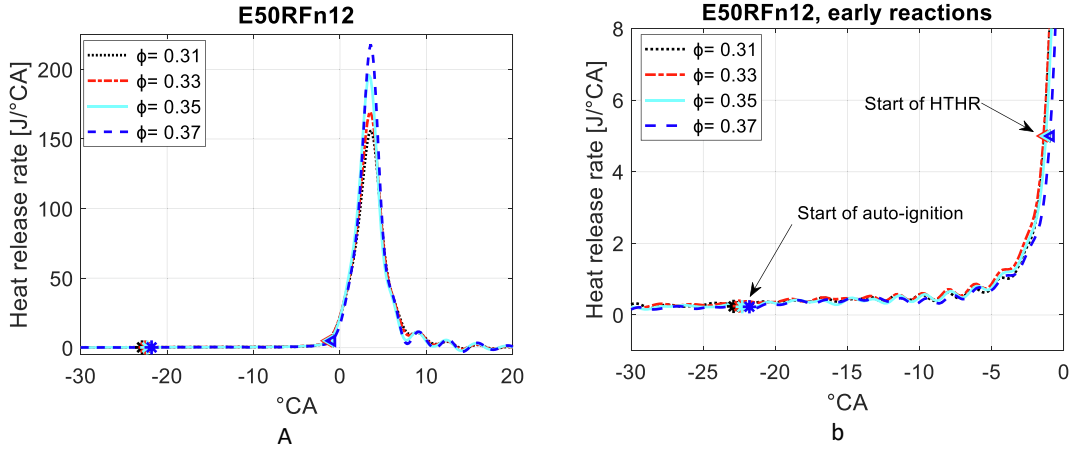

Fig. 9. HRR for the HCCI combustion of E50RFn12 at 323 K: a) complete HRR; b) HRR during the early reactions.

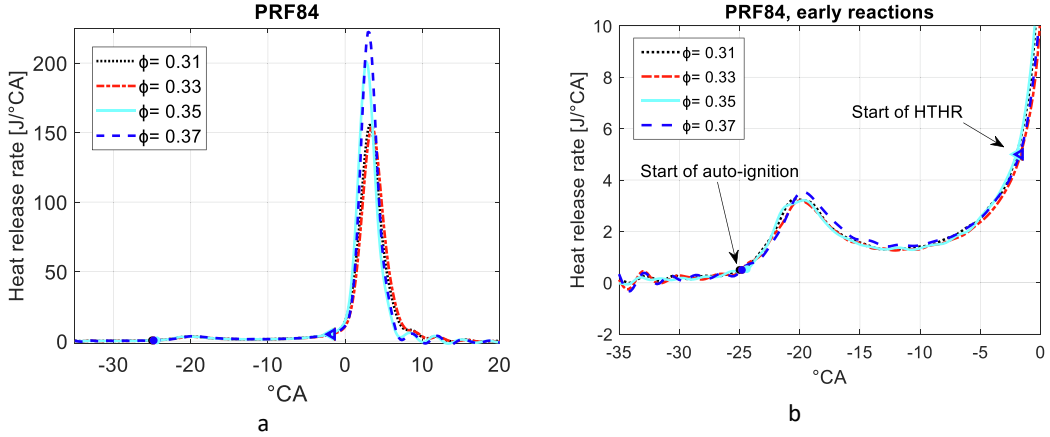

Fig. 10. HRR for the HCCI combustion of PRF84 at 323 K: a) complete HRR; b) HRR during the early reactions.

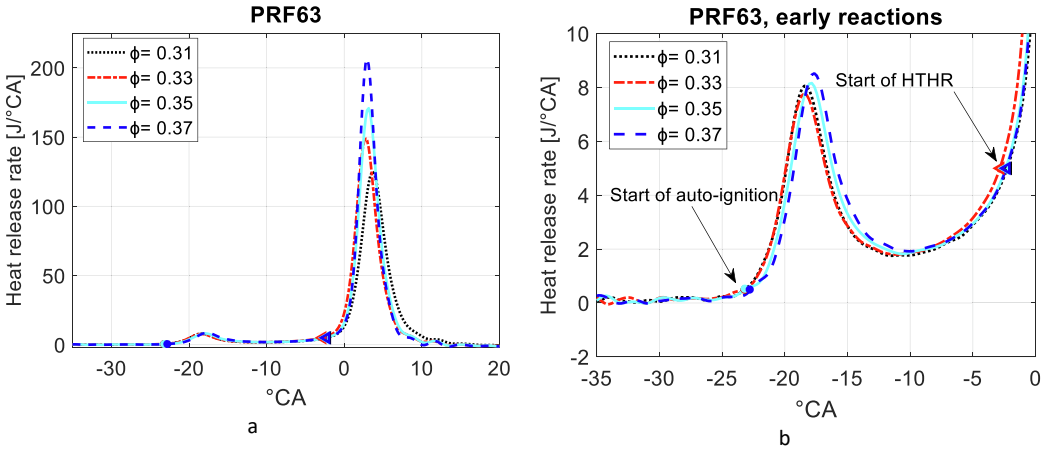

Fig. 11. HRR for the HCCI combustion of PRF63 at 323 K: a) complete HRR; b) HRR during the early reactions.

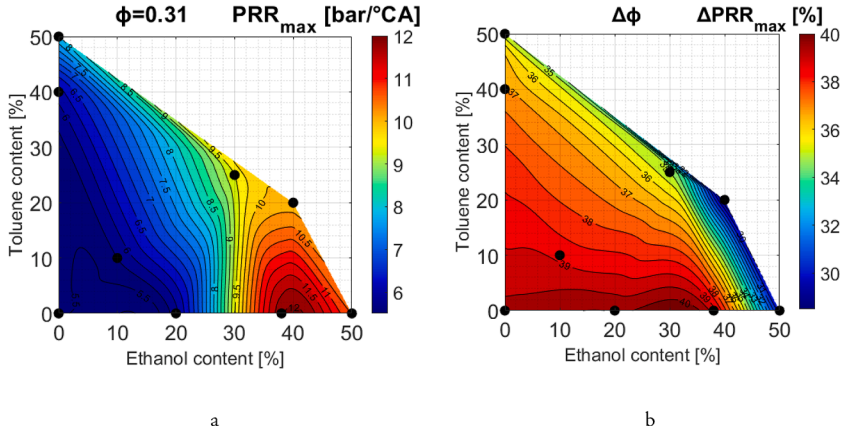

Fig. 12. (a) Maximum pressure rise rate (PRR_{max}) in the leanest condition as a function of ethanol and toluene content; (b) variation in PRR_{max} as a function of ethanol, toluene, and Δϕ.

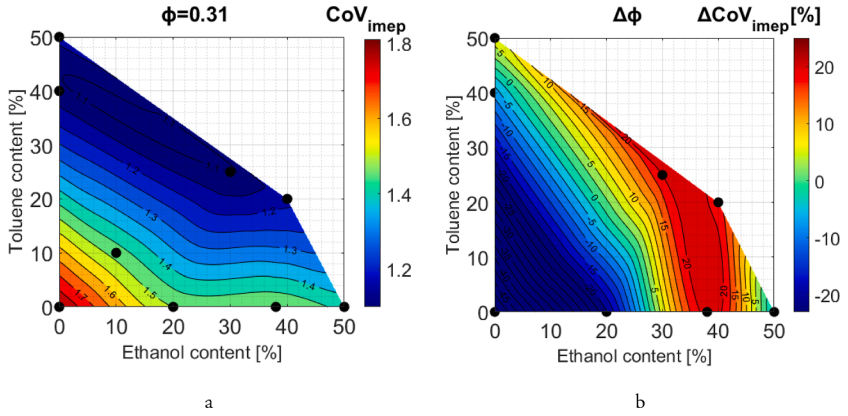

Fig. 13. (a) COV_{IMEP} in the leanest condition as a function of ethanol and toluene content; (b) variation in COV_{IMEP} as a function of ethanol, toluene, and Δϕ.

early reactions (Fig. 5) as well as the charge cooling effect of ethanol.

3.2. Combustion and auto-ignition behavior of different blends

As explained above, the studied TERFs are designed to have three different RONs of 105, 84, and 63. As a result of these different RONs, both single- and two-stage combustions can be investigated in the experimental results. The intake temperature for most of the results presented in this paper is 323 K and the engine speed for all of the operating points is 900 RPM. A recent study of the fuel ϕ-sensitivity suggests that the ITHR could be an indicator of the fuel ϕ-sensitivity [46], so any variation in ϕ should also affect the ITHR. Pintor et al. also explain that the amount of accumulated LTHR is unaffected by the phi sweep [46]. Fig. 9 shows the heat release profile of $E_{50}RFn_{12}$ as an example of the RON = 105 group. The plot shows that $E_{50}RFn_{12}$, which is an oxygenated high-RON fuel, does not exhibit any LTHR in naturally aspirated conditions and is a single-stage combustion fuel; however, its ITHR lasts for more than 20 CAD and accounts for only 1.2% of the

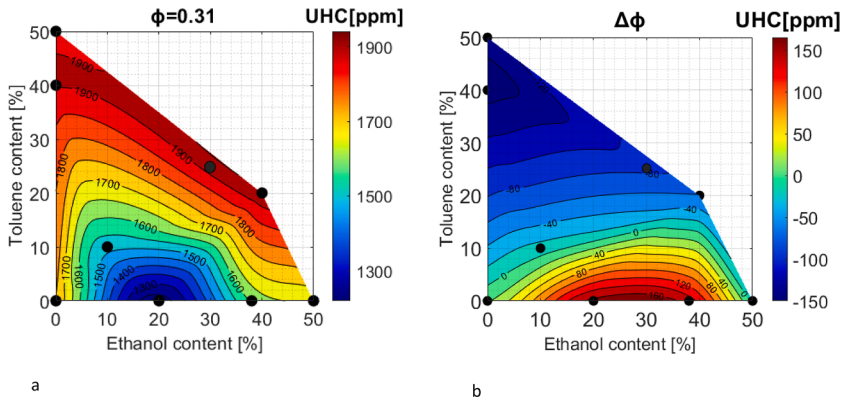

Fig. 14. (a) UHC emissions in the leanest condition; (b) the effect of ϕ increase on UHC reduction for different blends.

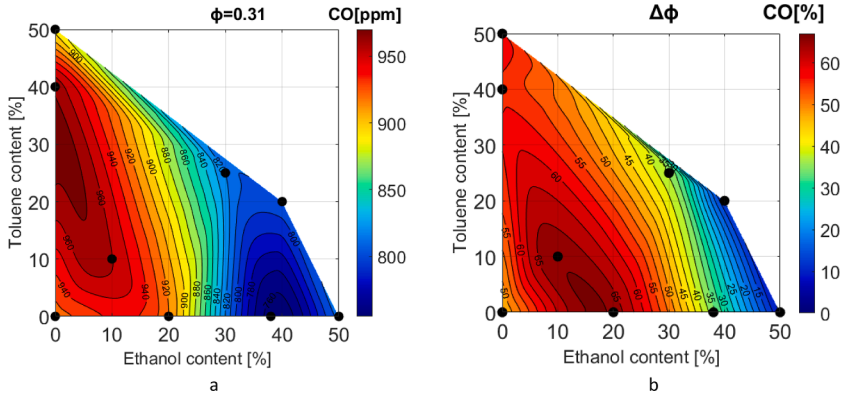

Fig. 15. CO emissions: CO emissions at a specific ϕ(left), effect of ϕ increase on the CO emission reduction for different blends(right).

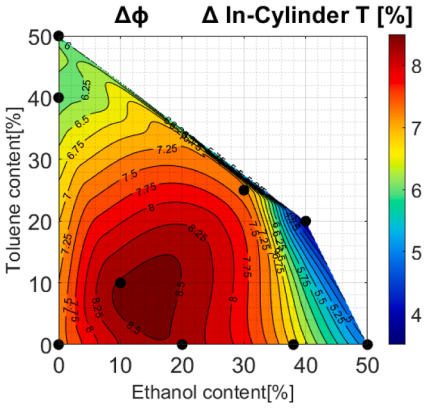

Fig. 16. Variation in maximum in-cylinder temperature due to the increase in ϕ.

TAcHR of this fuel at the different ϕ levels. While maintaining constant CA50 by compensating the effect from ϕ variation with variation of CR, the ITHR remained essentially unaffected.

The heat release profiles in Fig. 9 also demonstrate that although the early reactions and heat release are almost the same at all the phi levels of $E_{50}RFn_{12}$, the peak HRR for the highest ϕ of 0.37 is 30% greater than at the lowest ϕ of 0.31. This is due to the higher fuel mass in the combustion chamber and therefore the higher energy in the system. Note that to maintain constant combustion phasing at a higher ϕ, the CR needs to decrease.

Figs. 10 and 11 show the HRR for the two-stage combustion fuels. Fig. 10 shows the HRR for PRF84 as an example of the RON = 84 group. PRF84 is a binary reference fuel consisting of 84 V/V% iso-octane and 16 V/V% n-heptane with no oxygen content and zero octane sensitivity (S = RON – MON). Fig. 11 shows the HRR for PRF63 as an example of the RON = 63 group.

All blends in these two groups (i.e., RON = 84 and 63) have higher reactivity than do blends in the first group (i.e., RON = 105). Higher reactivity means that the fuel is more prone to auto-ignition and has a lower RON.

It can be observed from Figs. 10 and 11 that blends with RONs of 84 and 63 have clear two-stage combustion, with LTHR as well as ITHR. The heat released (both ITHR and LTHR) during the early reactions of PRF63 accounts for approximately 9.5% of the TAcHR for all the ϕ levels of this blend. For PRF84, the ITHR and LTHR account for approximately 6.5% of the TAcHR of the blend at the different ϕ levels. This shows that adjusting CR is a proper way to compensate the variation of amount of accumulated ITHR due to the ϕ variation for all of the two-stage combustions of both highly and moderately reactive blends.

3.3. Emission and stability parameters in relation with the ϕ variations

The joint effect of ϕ variation and fuel composition on the emissions was investigated to determine if the emissions could act as an indicator for the ϕ sensitivity. Such correlations are however too inconsistent. The results of the emission measurements can be found in appendix A. In this section, the joint effect of ϕ variation and fuel composition on the performance of the engine is presented and discussed.

3.3.1. Stability parameters in relation with the ϕ variations

The maximum pressure rise rate (PRR_{Max}) and coefficient of variation of indicated mean effective pressure (CoV_{IMEP}) are evaluated as the two parameters of combustion stability. Fig. 12a shows the PRR_{Max} of

the different blends in the leanest condition and at $T_{in} = 323$ K. Fig. 12a indicates that the blends with higher ethanol contents have more aggressive combustion with a higher PRR_{Max}. This could be due to the higher required CR in the leanest condition compared with the other blends in the same RON group (Fig. 3). All of the blends will increase their PRR_{Max} with increased ϕ (see Fig. 12b). This increase is due to the higher mass burn and higher energy in the system. The plots also show that adding toluene increases the PRR_{Max} at a slower rate than does adding the same percentage of ethanol.

Fig. 13a shows the CoV_{IMEP} in the leanest condition as a function of the ethanol and toluene contents. The low CoV_{IMEP} of this dataset shows that the engine is running stably throughout the experiments and yielding robust data. Fig. 13b shows the variation in CoV_{IMEP} due to the increase in ϕ. It can be concluded from this graph that adding an aromatic component is more effective in lowering the CoV_{IMEP} than is adding ethanol. The HCCI combustion stability response of different fuels to the ϕ variation is nonlinear.

4. Conclusion

The LTC concept is the basis for some of the high-efficiency, low-emission combustion technologies (e.g., HCCI, PPC, and RCCI). One of the most important properties which makes a fuel suitable for LTC is ϕ-sensitivity. High ϕ-sensitivity fuels have a smoother consequential combustion in case of fuel and/or thermal stratification. Moreover, using renewable drop-in fuels for combustion engines is suggested to be a practical approach for achieving reliable and sustainable transportation. The test method presented in this study, is an evaluation platform to tailor fuels with a preferable ϕ-sensitivity at a desirable RON. This study proposes an empirical method for ϕ-sensitivity evaluation, termed Lund ϕ-sensitivity number, which uses a conventional CFR fuel test engine to evaluate renewable fuels, conventional fuels, or any blends of conventional and renewable fuels, including compounds which do not have a detailed kinetic mechanism. The experiments demonstrate that the method provides a clear and consistent determination of ϕ-sensitivity for different fuels. The method is quick and doesn't rely on complex prerequisite data such as detailed kinetic mechanisms, which not always exist.

The following equation shows the way that the Lund ϕ-sensitivity number is calculated:

$$\text{Lund } \phi - \text{sensitivity} = \text{Norm CR} = -\frac{1}{\text{CR}}\frac{\Delta \text{CR}}{\Delta \phi}$$

The results of this evaluation show that:

- By maintaining constant combustion phasing (e.g., CA50) at different equivalence ratio (ϕ) levels of a fuel, the compression ratio (CR) variation can be interpreted as the ϕ-sensitivity indicator. CR variation signifies the ϕ-sensitivity of the fuel or blend. This approach can be used to quantify the ϕ-sensitivity of different fuels and blends with different RONs.
- This study suggests that the coexistence of oxygenated and aromatic hydrocarbons together with paraffins can maximize the Lund ϕ-sensitivity of the blends while maintaining RON at a desirable level.
- Adjusting CR to keep CA50 constant keeps the timing between the start of LTHR and the main combustion unchanged. CR adjustment during the ϕ sweep compensates for the effect of ϕ variation on the ignition delay variation and on the heat release ratio during early reaction to TAcHR.
- Fuel composition, independent of fuel RON, has a strong effect on the Lund ϕ-sensitivity of the fuel. Therefore, different fuels with the same RON can still have different Lund ϕ-sensitivities. Also, no correlation was found between emissions and Lund ϕ-sensitivity, but a clear correlation was found between emissions and blend compositions.
- There is a correlation between the heat release during the early reactions (ITHR + LTHR) and Lund ϕ-sensitivity number. This is in line with kinetic simulation studies by other researchers.
- The study suggest that there is a link between load adaptability of fuels and Lund ϕ-sensitivity number. Ethanol reference fuels has lower Lund ϕ-sensitivity number and load adaptability while Toluene-ethanol reference fuels with the same octane number have higher Lund ϕ-sensitivity number and higher load adaptability. Generally both Lund ϕ-sensitivity number and load range are higher for the blends with aromatic content.
- No robust correlation between the Lund-Chevron HCCI number, Octane sensitivity, heat of vaporization and Lund ϕ-sensitivity number was found in this study.

CRediT authorship contribution statement

Nika Alemahdi: Investigation, Formal analysis, Software, Visualization, Writing – original draft. **Antonia García-Martínez:** Supervision, Writing – review & editing. **Emma Boufaim:** . **Giulia Aferiat:** Investigation. **Martin Tunér:** Supervision, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A:

Carbon monoxide (CO), nitrogen oxides (NOx), particulate matter (PM), and unburned hydrocarbons (UHC) are the regulated tailpipe emissions of automotive engines. Due to lean and homogeneous LTC, the levels of thermal NOx are very low and PM formation does not occur [49,82–84]. Since this experiment was conducted in HCCI combustion mode, the NOx level did not exceed 60 ppm, so it is not further evaluated in this paper.

Unburned hydrocarbon (UHC) emissions

HCCI engines emit higher levels of unburned hydrocarbons (UHC) than of other types of legislated emissions. The main reason for high UHC emissions from HCCI combustion is the existence of homogeneous charge in the crevices during the combustion stroke. This trapped mixture does not burn and causes high levels of UHC emissions in the exhaust. Different studies show that even at a higher global in-cylinder temperature, the effect of the crevice volume is dominant [18,49,82]. In this study, CA50 was kept constant despite the ϕ variations; as explained above, this was achieved by adjusting the CR. When the ϕ was increasing, the CR required to keep the CA50 constant needed to be decreased. Therefore, the ratio of crevice volume to total in-cylinder volume decreases and, as a result, the UHC related to the crevice volume will also decrease. Fig. 14 shows the UHC emissions of all of tested blends. Fig. 13b shows the variation in UHC when the ϕ increases. Blends with aromatic content display a decrease in UHC emissions in response to an increase in ϕ. When ethanol is the only source of octane

sensitivity (S) in the blends, this expected decrease in UHC emissions no longer occurs. The ethanol content of the blends starts affecting the UHC, changing the pattern from the low level of 10 V/V%. This effect is mainly due to the charge cooling effect of oxygenated blends. Table 2 shows that the heat of vaporization (HoV) of the oxygenated blends is significantly higher than that of the non-oxygenated blends.

As an example in the RON 63 group, only 10% ethanol in $T_{10}E_{10}RFn_{49}$ sets the HoV at 376, which is 12% higher than that of $T_{40}RFn_{48}$ and 21% higher than that of PRF63, which have HoV values of 332.9 and 310, respectively, and are the non-oxygenated blends in this group. The important point to consider is that despite this effect, oxygenated blends generally emit less UHC than do other fuels with the same RON, due to the oxygen content of the blends. It can be concluded that both the UHC level and UHC variation pattern are due to the ϕ variation, which is highly dependent on the fuel composition.

Carbon monoxide (CO) emissions

Fig. 15 shows the CO emission level for each blend in the leanest condition as well as the effect of ϕ variation on the CO emission reduction for different blends. The oxygenated blends emit less UHC and CO than do the other blends at the same ϕ. The reason for the lower UHC and CO emissions is the improved combustion due to the oxygen content of the blends [6,48,74,85]. In this study, all of the blends display a decrease in CO emissions due to the increase in ϕ. In Fig. 15b, the percentage of CO variation is multiplied by (–1) to avoid negative values.

For all the blends, a higher ϕ lowers the CR required to keep the CA50 constant, but since the ϕ increases by means of an increase in fuel mass, the in-cylinder temperature does not drop as if the ϕ was constant. Fig. 16 shows the percentage increase in maximum in-cylinder temperature due to the ϕ increase. As expected, the blends that cause less increase in maximum in-cylinder temperature also result in a smaller decrease in CO emissions due to the ϕ increase.

As this section demonstrates, the emissions of the ϕ sensitivity experiments are directly influenced by the fuels compositions and the engine geometries as well as CR and in cylinder temperature. To be able to study the effect of fuel's ϕ sensitivity number on emission formation other experiments must be designed in a way that isolates the effect of the variation of CR and the ratio of crevice volume to the total in-cylinder volume. Such experiments were not in the scope of this study, but would definitely be interesting to perform in future works.

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