2023-01-0251

Development of a Supercharged Octane Number and a Supercharged Octane Index

Author, co-author (Do NOT enter this information. It will be pulled from participant tab in MyTechZone)
Affiliation (Do NOT enter this information. It will be pulled from participant tab in MyTechZone)

Abstract

Gasoline knock resistance is characterized by the Research and Motor Octane Number (RON and MON), which are rated on the CFR octane rating engine at naturally aspirated conditions. However, modern automotive downsized boosted spark ignition (SI) engines generally operate at higher cylinder pressures and lower temperatures relative to the RON and MON tests. Using the naturally aspirated RON and MON ratings, the octane index (OI) characterizes the knock resistance of gasolines under boosted operation by linearly extrapolating into boosted "beyond RON" conditions via RON, MON, and a linear regression K factor. Using OI solely based on naturally aspirated RON and MON tests to extrapolate into boosted conditions can lead to significant errors in predicting boosted knock resistance between gasolines due to non-linear changes in autoignition and knocking characteristics with increasing pressure conditions. A new "Supercharged Octane Number" (SON) method was developed on the CFR engine at increased intake pressures, which improved the correlation to boosted knock-limited automotive SI engine data over RON for several surrogate fuels and gasolines, including five "Co-Optima" RON 98 fuels and an E10 regular grade gasoline. Furthermore, the conventional OI was extended to a newly introduced Supercharged Octane Index (OI_S) based on SON and RON, which significantly improved the correlation to fuel knock resistance measurements from modern boosted SI engine knock-limited spark advance tests. This demonstrated the first proof of concept of a SON and OI_S to better characterize a fuel's knock resistance in modern boosted SI engines.

Introduction

Today's carbon dioxide (CO_2) emissions targets for internal combustion engines are regulated by most governments worldwide [1, 2]. Spark ignition (SI) engines usually improve efficiency and performance by increasing compression ratio, down-speeding, and downsizing in combination with turbocharging, which operates the engine in a more efficient part of the operating map resulting in lower vehicle fuel consumption. Yates et al. showed how a switch from carbureted to fuel-injected engines shifted the cylinder pressure-temperature trajectory toward relatively higher pressure and lower temperature, Figure 1. Yates et al. furthermore showed that turbo- or supercharged engines increased the cylinder pressure-temperature trajectory even further into the "Beyond RON" region (green) [3]. While Yates et al. attribute this trend to the fueling technology, it is likely that improved engine breathing technologies, including the implementation cam phasers, significantly contribute to this trend. These technological advancements increase the propensity for gasolines to autoignite during the compression or combustion strokes of the engine. Autoignition is governed by the available time at kinetically active pressures and temperatures. Autoignition of the air-fuel mixture causes multiple flame fronts with local high heat release rates within the combustion chamber, subsequently creating superimposed high-frequency pressure oscillations called "knock". Knocking combustion can damage the combustion chamber and therefore limits the performance and efficiency of a spark-ignited internal combustion engine.

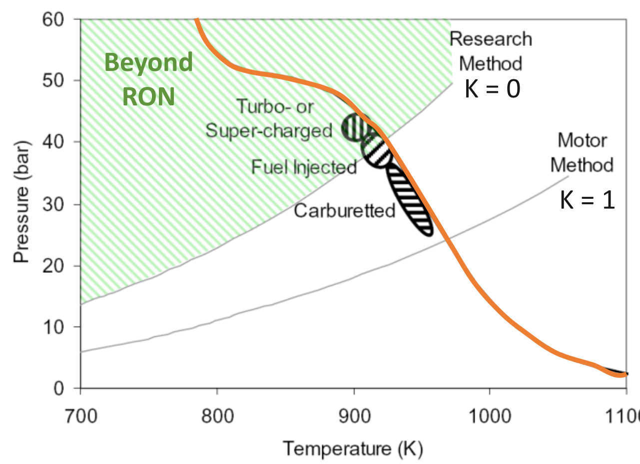

Figure 1. Pressure-temperature trajectories of the RON and MON methods relative to auto-ignition zones for different engine technologies and a constant ignition delay contour line (orange). Reprinted with permission from Yates et al. [3]. © SAE International.

The standard measurements of knock resistance of gasoline are the Research and Motor Octane Numbers (RON, MON). The RON and MON ratings are performed on a Cooperative Fuels Research (CFR) engine at defined operating conditions following ASTM D2699 and D2700 methods, respectively [4, 5]. Table 1 summarizes the operating conditions of RON and MON while Table 2 provides important engine parameters of the CFR engine. The CFR engine is a single-cylinder internal combustion engine designed to withstand harsh knocking combustion and is equipped with a unique variable compression ratio system that allows continuous compression ratio adjustment even while the engine is firing or knocking. The CFR engine is operated under naturally aspirated conditions. The RON test is conducted at lower engine speeds and intake air temperatures compared to MON [4, 5]. Yates et al. calculated the pressure-temperature trajectories of RON and MON operation relative to the development of engine technology, Figure 1 [3]. Pulpeiro et al.

showed how the pressure-temperature trajectories of standard RON and MON operations can differ depending on the calculation methodology [6]. While these uncertainties remain, the RON tests create higher cylinder pressures for a given temperature compared to MON, but not as high as modern boosted SI engines.

Table 1 Overview of operating conditions for RON and MON ratings [4, 5]

Parameter	RON	MON
Engine Speed	600	900
Intake Air Temperature	52 °C	38 °C
Mixture Air Temperature	Not controlled	149 °C
Spark Timing	13 °bTDC	Variable, depending on compression ratio
Lambda	Peak Knock	Peak Knock
Intake Pressure	Naturally aspirated	Naturally aspirated
Compression Ratio	Based on octane level and barometric pressure	Based on octane level and barometric pressure

Table 2 Overview of CFR Engine geometric parameters [4, 5]

Parameter	CFR Engine
Displacement	0.612 cc
Cylinder Bore	8.255 cm
Stroke	11.43 cm
Compression Ratio	Continuously variable from 4:1 to 18:1
Fuel System	Carbureted with four fuel bowls
Intake Valve	One shrouded non-rotating valve
Exhaust Valve	One non-shrouded rotating valve
Valve Overlap	5 CAD
Combustion Chamber Geometry	Pancake
Spark Plug	Side-mounted

The CFR engine, along with the RON and MON methods, were developed in the early 1930s and therefore differ somewhat from modern engine operation [7-10]. In 1932, MON had a superior correlation to on-road fuel performance. Advances in engine technology such as better engine cooling systems shifted the relevance to RON [11]. In 2001, Kalghatgi introduced the Octane Index (OI), which established a linear trendline with RON and MON as boundaries, equation 1 [12]. The OI generates superior correlations over RON and MON due to the engine operation-specific factor K, which represents the slope between RON (K=0) and MON (K=1).

$$OI = RON - K * (RON - MON) \quad (1)\ [12]$$

Mittal et al. investigated the evolution of the K-factor distribution and showed that historically, engines had a K-factor around 0.5, which would equate to the average of RON and MON and is termed the anti-knock index (AKI) [11]. The anti-knock index is used as the most common fuel rating for commercial gasoline sales in the United States. Mittal et al. also showed that naturally aspirated spark-ignited engines from the 2008 timeframe had a K value close to 0, meaning RON was more representative than MON. Furthermore, spark ignition engines with forced induction tended toward negative K-factors, around -0.5 [11]. This indicates an OI extrapolation outside of the RON-MON boundaries and can introduce uncertainties. Linear extrapolation is especially challenging when coupled with non-linear physical phenomena. The previously shown pressure-temperature trajectories in Figure 1 originally published by Yates et al. also show a contour line of constant ignition delay time (orange) [3]. Yates et al. determined this constant ignition delay contour for a typical market gasoline with a RON-MON sensitivity of 10. While mostly following a linear trendline between RON and MON, the ignition delay contour line shows significant non-linearities at pressures higher than the RON pressure-temperature trajectory in the beyond RON region [3]. These non-linearities of ignition delay are coupled with the fuel's chemical composition [13]. Primarily paraffinic fuels experience a negative temperature coefficient (NTC) behavior which is a non-linear increase in ignition delay times with an increase in temperature [3, 14].

Mittal et al. discussed changes to the RON and MON methods to realign the boundaries for the OI calculation toward higher pressures. He suggested an intake air pressure of 1.4 bar(a), 900 rpm engine speed, and 30 °C intake air temperature for the RON test, as well as 1 bar intake pressure, 1500 rpm engine speed, and 70 °C intake air temperature for the MON test. These would shift the pressure-temperature trajectories to again bracket those of modern boosted engine operation [15]. While those changes were proposed, they have not been introduced by the ASTM committee, nor tested on a CFR engine. One likely reason could be the significant impact on worldwide octane assessment and accompanying changes to the gasoline distribution network to ensure compliance with the octane standards. DelVescovo and Salih followed a similar approach to Mittal but introduced a newly developed Boosted Octane Number in addition to standard RON and MON methods. Based on GT-Power simulations, two Boosted Octane Number test methods were suggested, both at increased intake pressure, increased engine speed, and reduced intake temperature [16].

Both DelVescovo and Mittal suggested excellent changes to the octane test on a CFR engine to better align the pressure-temperature characteristic to modern boosted engine operation [15, 16]. However, neither work had the opportunity to collect experimental data to validate the simulation results. This work upgraded a standard RON-MON CFR engine to allow for data collection of experimental octane tests at elevated intake pressures. Furthermore, the fuel matrix was selected to allow for knock rating comparisons to a knock-limited modern boosted gasoline direct-injection (GDI) engine, which subsequently validates the newly developed Supercharged Octane Number (SON) over the standard RON rating. This work also introduces a newly developed Supercharged Octane Index (OI_S) that follows the methodology of the original OI but replaces the interpolation brackets of RON and MON for RON and SON, leading to an improved correlation to modern boosted GDI engine operation. The objective of this study is to introduce the framework for a new Supercharged Octane Number test methodology and provide proof of concept, which ideally will lead to the further development and refinement of the test method to eventually become an official test standard.

Methodology

The development process of this work started with data acquisition system upgrades to a conventional CFR engine. Furthermore, a compressed air intake system was developed and validated via Fit for Use tests. The newly developed compressed air intake system enabled engine operation at supercharged intake pressures, which required modifications to the carburetor fuel system. After highlighting shortcomings of the conventional octane assessment, CFR engine operation parameters for a Supercharged Octane Number (SON) test and respective test fuels were selected. An alternative SON test method was performed before the conventional OI was extended to a OI_S. The following sections will provide a detailed description of each development milestone.

Experimental Procedures

All SON experiments were conducted on a CFR engine. Before any engine upgrades were performed, the engine passed the motoring peak pressure test and Fit for Use requirements based on the ASTM RON method [4]. For standard octane tests, the knock intensity of a sample fuel is compared relative to primary reference fuels (PRF). PRFs are a binary blend of iso-octane and n-heptane, with a defined octane number equal to the volumetric percentage of iso-octane. The knock intensity during a standard octane test is characterized by a standardized knockmeter system, which consists of a D1 Detonation Pickup, a 501C Detonation Meter, and a Knockmeter scale [4]. All data points were collected at steady-state operation for 300 consecutive cycles.

CFR Engine Upgrades

A standard CFR F-1 octane rating engine was upgraded to allow for the development of a Supercharged Octane Number. In the first step, the engine was outfitted with a LabVIEW-based data acquisition system to monitor intake and exhaust temperatures and pressures, as well as relative humidity in the intake manifold. The engine was also outfitted with modern combustion research tools such as a wide-band lambda sensor and a spark plug cylinder pressure transducer. Table 3 and previous publications provide a more detailed overview of the utilized instrumentation [17-19].

Table 3. Combustion research measurement and instrumentation systems employed on the CFR engine at Argonne National Laboratory.

Crankshaft angle-based measurements	
Crank-angle-based DAQ	AVL IndiCom & crankshaft encoder with 0.1 CAD resolution
Spark timing	Current clamp on coil wire
Intake pressure	Kulite flush-mounted uncooled high-speed 2.0 bara pressure transducer
Exhaust pressure	Kulite flush-mounted water-cooled high-speed 3.5 bara pressure transducer
Cylinder pressure	AVL GU13Z-24 flush-mounted spark plug pressure transducer
Time-based measurements	
Time-based DAQ	LabVIEW
Intake pressure	Setra 3550 pressure transducer
Exhaust pressure	Setra 3550 pressure transducer
Intake, mixture, exhaust, coolant, and oil temperature	K-type thermocouples
Fuel rate	Emerson CMF010M Coriolis Meter
Lambda	Bosch wide-band lambda sensor LSU 4.9
CFR knock units	Data-logged knockmeter signal

The standard CFR engine is equipped with a carburetor and is designed to operate at naturally aspirated conditions. Rockstroh et al. designed and implemented a compressed air intake system for the CFR engine in a previous publication [20]. Figure 2 shows the CFR engine setup with the components of the compressed air intake system. Dry, oil-free, and filtered compressed air is supplied to the engine and the pressure is regulated by an Alicat mass flow controller before entering the intake manifold 6” diameter transfer tube. The system also contains a pressure relief and a vacuum check valve to safeguard the pressure range in the manifold. Due to limitations of the standard sealing surfaces throughout the intake manifold, the intake pressure was limited to a maximum of 1.5 bar(a).

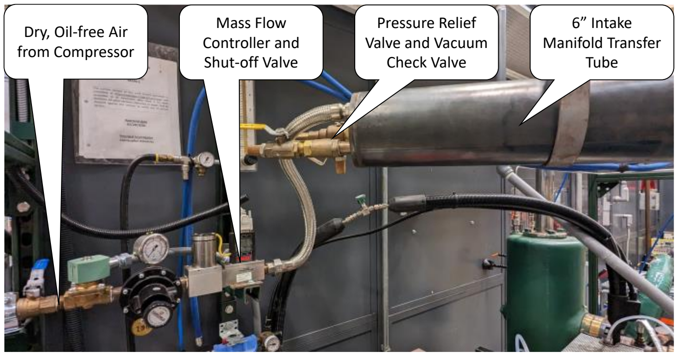

Figure 2. Compressed air intake manifold for a CFR engine.

A carburetor works based on a pressure differential in a venturi to pull fuel into the air stream. Therefore, when increasing the intake air pressure, the fuel pressure needs to match the air pressure for the carburetor to remain functional. The carburetor is retained instead of switching to a fuel injector at this stage to allow for the least amount of modifications to the CFR fueling system. Figure 3 shows a schematic of the added line routing for the carburetor (green). All conventional ventilation holes were connected to the intake manifold surge tank while the fuel bowl was sealed and also connected to the intake manifold surge tank.

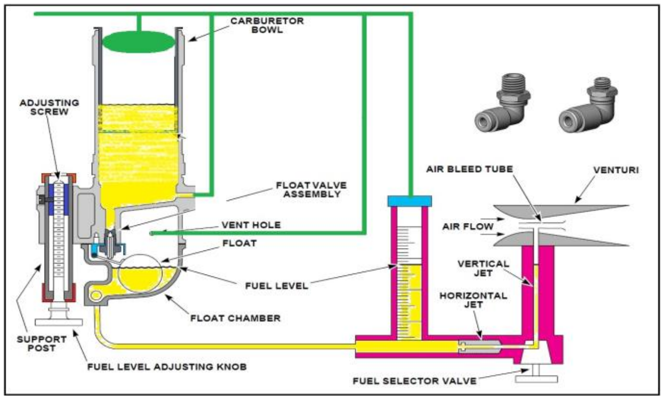

Figure 3. Carburetor line routing for operation at elevated intake and fuel pressures

The applied engine modifications did not change the geometry of the intake, exhaust, or combustion chamber. This ensured the best possible consistency with the standard CFR engine. To validate the compressed air intake system, a motored peak pressure test and a Fit for Use test following the standard ASTM D2699 RON method were conducted for multiple toluene standardization fuels (TSF) and passed the requirements without requiring temperature tuning.

Engine Operating Conditions

The initial Supercharged Octane Number (SON) testing in the CFR engine was performed at a range of intake pressures and otherwise standard RON settings, such as 52°C intake temperature and 600 rpm engine speed. The final intake pressure as well as two different SON test variants and other details such as knock intensity characterization and equivalence ratio for SON testing are discussed in the Results and Discussion section.

Szybist et al. also performed knock-limited combustion phasing tests in a modern boosted GDI engine, which was converted from multi- to single-cylinder operation [21]. This study extracted the knock-limited crank angle of 50% mass fraction burned (KLCA50) data from Szyist et al. engine operation at 2000 rpm engine speed, 50 °C mixture air temperature, and 1.5 bar absolute manifold air pressure conditions [21]. The knock-limited boosted engine operation data from Szybist et al. is used to validate the SON test results in the Results and Discussion section. Table 4 provides an overview of engine operating conditions for the SON tests on the CFR engine and the knock-limited boosted operation by Szybist et al. Note that all intake pressures throughout this paper are shown in bar absolute.

Table 4. Overview of engine operation conditions for Supercharged Octane Number testing on the CFR engine and comparison to engine test conducted by Szybist et al [*21*]

Parameter	**CFR Engine SON Testing**	**Szybist et al. GDI Testing [21]**
Intake Pressure	1 – 1.5 bar	1.54 bar
Intake Temperature	52°C	50 °C
Engine Speed	600 rpm	2000 rpm
IMEP	7 – 12 bar	15 – 20 bar

Fuel Selection

This study used primary reference fuels (PRF) and toluene standardization fuels (TSF) from the standard octane test methods, along with several full-boiling range gasolines. During the fuel matrix design, it was important to select fuels that had experimental data available from knock-limited boosted GDI operation. Table 5 provides a fuel summary with octane numbers and chemical compositions. Four PRFs ranging from PRF 90 to PRF 100 were used as reference fuels to bracket the knock characteristic of the sample fuels. PRFs are fully paraffinic fuels and have a defined octane number equal to the volumetric concentration of iso-octane in a binary blend with n-heptane. Therefore, PRFs are defined to have a RON-MON sensitivity of 0. In addition, a TSF with a defined composition and a RON of 96.9 was used. TSFs are highly aromatic fuels and are used to ensure CFR engine compliance with the RON and MON methods.

A study by Szybist et al. explored the knock-limited combustion phasing of numerous gasolines [21]. Of those fuels, this study selected five core fuels of the Co-Optimization of Fuels & Engines (Co-Optima) program [22]. The Co-Optima fuels have a target RON of 98 but vary noticeably in their chemical composition. The primarily paraffinic alkylate gasoline (RON98Alk) has a minimal RON-MON sensitivity while the other four Co-Optima gasolines have a
RON-MON sensitivity of around 10 and are getting their sensitivity from either aromatics (RON98Aro), cycloalkanes (RON98CA), ethanol (RON98E30), or olefins (RON98Ole). In addition, the EPA Tier 3 EEE certification gasoline for regular octane grade with 10 vol% ethanol was selected to be representative of market gasoline.

Table 5. Overview of test fuel composition and octane numbers
* – Composition based on detailed hydrocarbon analysis

Fuel	RON	MON	Composition [vol%]		
			Iso-octane	n-Heptane	Toluene
PRF100	100	100	100	0	0
PRF96	96	96	96	4	0
PRF93	93	93	93	7	0
PRF90	90	90	90	10	0
TSF96.9	96.9	85.2	5	21	74
RON98Alk*	97.9	96.7	n-Paraffin: 3 Aromatics: 1 Olefins: 0	Iso-Paraffin:96 Naphthenes: 0 Ethanol: 0	
RON98Aro*	97.9	87.3	n-Paraffin: 8 Aromatics: 40 Olefins: 5	Iso-Paraffin:38 Naphthenes: 8 Ethanol: 0	
RON98CA*	97.6	86.6	n-Paraffin: 8 Aromatics: 33 Olefins: 2	Iso-Paraffin:32 Naphthenes: 24 Ethanol: 0	
RON98E30*	97.6	87.6	n-Paraffin: 13 Aromatics: 14 Olefins: 6	Iso-Paraffin:28 Naphthenes: 7 Ethanol: 30	
RON98Ole*	98.5	87.8	n-Paraffin: 12 Aromatics: 13 Olefins: 27	Iso-Paraffin:44 Naphthenes: 3 Ethanol: 0	
Tier 3 EEE	92.1	84	Saturates: 63 Olefins: 6	Aromatics: 23 Ethanol: 10	

Results and Discussions

Shortcomings of Conventional Octane Assessment

Literature shows, that there is a discrepancy between a fuel's RON rating and its knock-limited performance in boosted GDI engines [9-11, 17, 21, 23]. A previous study by the authors compiled knock-limited combustion phasing data from RON-like operation of RON98 gasoline in modern engines, which revealed significant discrepancies depending on the fuel's chemical composition [17]. Correlations to knock-limited data from modern boosted engine operation show even higher discrepancy to octane ratings. Figure 4 shows the correlation between the KLCA50 data from Szybist et al., which was taken at 1.5 bar intake pressure in a modern boosted engine (cf. Table 4), and the standard RON rating of the fuels. A linear trendline was added and its coefficient of determination (R^2) is extremely poor. The knock-limited combustion phasing seems completely independent from the RON ratings. The Tier 3 EEE with a RON rating of 92.1 had the same KLCA50 as PRF100 and RON98Alk, which both have a significantly higher RON. However, it is noteworthy, that both PRF100 and RON98Alk are highly paraffinic. Previous publications by the authors and others have shown paraffinic compounds to have high knocking cylinder pressure oscillations for a given RON rating, which would contribute to a delayed knock-limited combustion phasing based on a constant knock intensity threshold [17, 18, 23, 24]. The TSF96.9 also stands out due to its advanced KLCA50 based on its RON rating compared to the other fuels. As mentioned in the Fuel Selection section, TSF96.9 is highly aromatic and aromatics have been shown to reduce the cylinder pressure-based knock intensity for a given RON [17, 18, 23, 24].

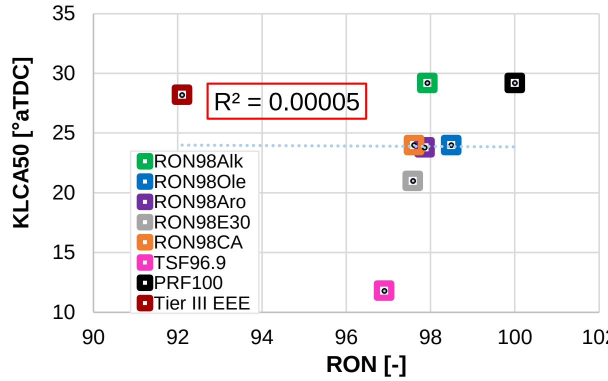

Figure 4. KLCA50 correlation to RON. KLCA50 data from Szybist et al. at 2000 rpm, 40 °C, 1.5 bar intake pressure [21]

OI allows for a better characterization of the knock resistance of gasoline since the K-factor can be iterated to achieve an optimal correlation. To some degree, the K-factor also describes where in the pressure-temperature space the engine operates relative to RON and MON. Figure 5 shows the same KLCA50 data from Figure 4, but plotted against OI on the x-axis. The OI significantly improved the correlation by aligning the fuels closer to the plotted trendline. This trendline suggests an advanced KLCA50 rating for fuels with an increased OI, which is the expected trend. TSF96.9 still outperformed its expected KLCA50, which reduced the coefficient of determination and hence only allowed for a mediocre correlation ($R^2 = 0.52$). The PRF100 had the highest RON rating of all tested fuels, but it also had the lowest OI in Figure 5 along with RON98Alk due to their low RON-MON sensitivity. All other fuels had a significant RON-MON sensitivity. For a negative K-factor such as in Figure 5, the RON-MON sensitivity adds to the knock-resistance of the fuel making it more knock resistance with a lower MON for a given RON, which also shifts the OI into the beyond 100 range. A negative K value also means an extrapolation outside of the RON-MON boundaries towards the beyond RON region, which is characterized by increased pressure for a given temperature. This aligns with the testing conditions at elevated intake pressure by Szybist et al. and previously discussed findings from Mittal et al. and Yates et al. [3, 10, 15, 21]. Adding one additional reference point of a Supercharged Octane Number can be beneficial in reducing the required extrapolation outside of RON and MON.

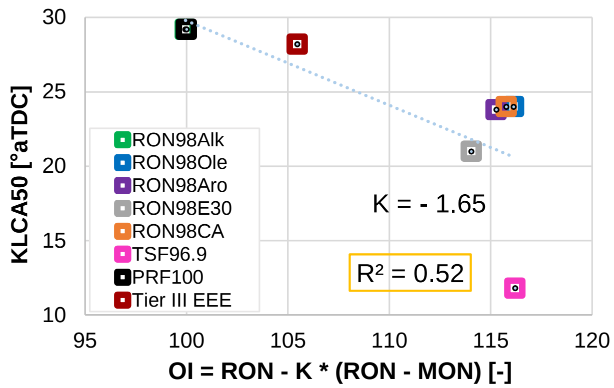

Figure 5. KLCA50 correlation to OI with K optimized for best R2. KLCA50 data from Szybist et al. at 2000 rpm, 40 °C, 1.5 bar intake pressure [21]

Supercharge Octane Number Test Method

The Supercharged Octane Number (SON) test method proposed in this work utilized the variable compression ratio of the CFR engine and follows a similar approach to Procedure C, compression ratio method of the ASTM D2699 RON method [4]. The compression ratio is adjusted for each fuel until a knock intensity threshold is met. During standard RON testing, the knock intensity is quantified using a standardized knockmeter system. However, there are concerns about the capability of the CFR knockmeter system to respond to high-frequency pressure oscillations [17, 18, 23, 24]. Therefore, a knock intensity threshold based on cylinder pressure oscillations was selected instead, which was the same knock intensity measurement technique used to determine the KLCA50 of each fuel on the modern boosted GDI research engine [21]. On the CFR engine, the cylinder pressure captured by the spark plug pressure transducer is first filtered for knock resonant frequencies in a range from 4 to 18 kHz and then rectified. The maximum of the filtered and rectified pressure signal is evaluated for each cycle and then averaged across 300 consecutive cycles to calculate the maximum amplitude of pressure oscillations (MAPO). A knock intensity threshold of 0.6 bar MAPO was selected for all data points of this study, which allowed for knocking combustion of each cycle. Literature and previous work by the authors showed that the standard CFR knockmeter system filters out high-frequency content, but Swarts et al. showed that the D1 Detonation Pickup is capable of capturing a MAPO-like signal and could potentially be used instead of the cylinder pressure-based MAPO knock intensity threshold [18, 23, 24]. For the standard RON test, the lambda is adjusted for peak knock intensity. Modern engines usually operate at stoichiometry. To ensure the maximum applicability of a new octane test to on-road engine operation, stoichiometric operation was selected for the SON testing. The authors published multiple papers on the effects of shifting lambda from peak knock to stoichiometry [17,18]. The spark timing (ST) of 13°bTDC, the engine speed of 600 rpm, and the intake air temperature of 52 °C from the standard RON method were retained for the SON testing, Table 4 [4].

Figure 6 shows the required compression ratio results for all fuels across varying intake pressures to meet the knock intensity threshold at stoichiometric operation and constant spark timing. This is the foundation of the SON test method and indicator of a fuel's knock resistance. Overall, a lower compression ratio is required when increasing the intake pressure. Spotting fuel-specific trends in this first stage of the SON results is challenging due to the wide range of compression ratios. It is however noted, that TSF96.9 exceeded the required compression ratio of iso-octane, which is designated as PRF100. Iso-octane is defined as 100 on the octane scale and sets the upper limit of binary blends with n-heptane. PRFs higher than 100 are blends of iso-octane and tetraethyl lead (TEL) but were not used in this study.

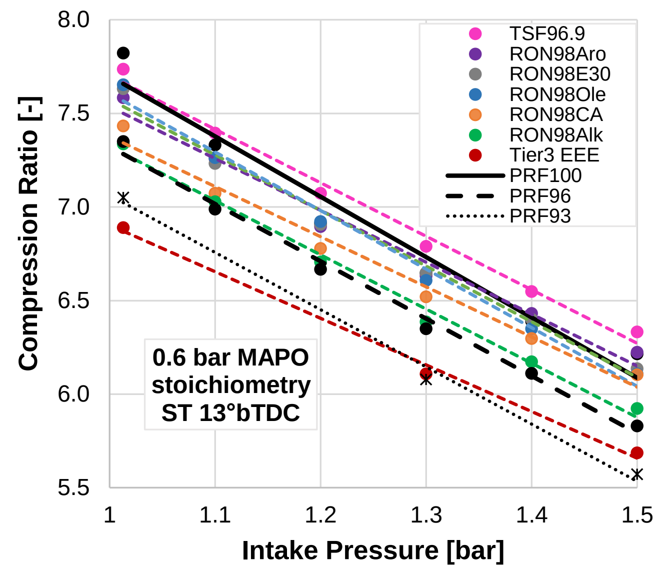

Figure 6. Critical compression ratios at varying intake pressures.

The standard RON Procedure C uses PRFs to bracket the compression ratios of sample fuels [4]. An identical approach was used for the calculation of SON in this study. The compression ratio of a sample fuel is bracketed by the compression ratio of two PRFs at the same intake pressure conditions. This also implies that the SON of PRFs is equal to the concentration of iso-octane, following the RON and MON methodology. Figure 7 shows the calculated SON of all test fuels at varying intake pressures. It is noted that all fuels showed an increased SON with higher intake pressures. This follows in part the OI methodology which suggests that fuels with higher RON-MON sensitivity should have an increased knock resistance at higher intake pressures. Most notably, Tier 3 EEE stands out with a significant increase in SON for higher intake pressures. However, Tier 3 EEE only has a mid-range RON-MON sensitivity compared to most other test fuels. Furthermore, the RON98Ole gasoline with a RON-MON sensitivity close to 11 only showed a slight increase in SON, similar to RON98Alk, which had a RON-MON sensitivity of only 1.2. It is also noted, that TSF96.9 and RON98Aro exceeded an SON of 100, being more knock resistant than iso-octane. To calculate the SON greater than 100 for TSF96.9, an extrapolation was performed based on the MAPO knock intensities of PRF96 and PRF100. Notably, PRFs are known for their NTC behavior and low-temperature chemistry at higher intake pressures. This could explain why iso-octane was less knock resistant at high intake pressures than highly aromatic fuels with lower RON [3, 14, 25].

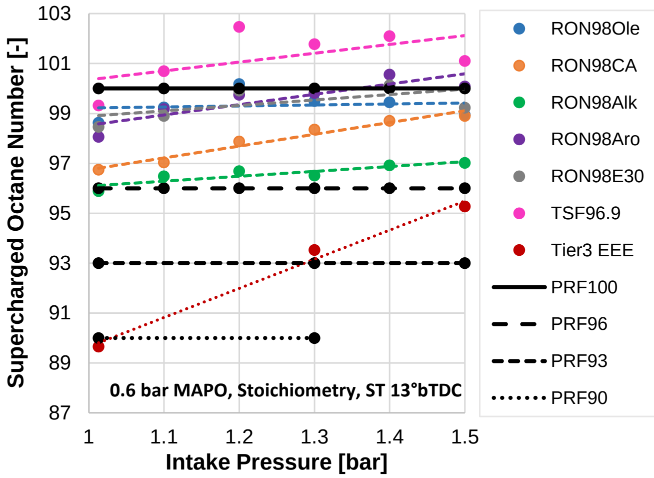

Figure 7. Supercharged Octane Number trends for varying intake pressures

The intake pressure during SON testing was limited to 1.5 bar(a) because of limitations of the carburetor system and the sealing surfaces in the intake manifold. For further correlations to KLCA50 data, the highest intake pressure condition was selected for SON testing since it provided the greatest pressure increase in terms of pressure-temperature trajectory from the standard RON test. Furthermore, the experimental data from Szybist et al. was also collected at 1.5 bar intake pressure. However, Szybist et al. used a higher engine speed (2,000 rpm) compared to the SON testing on the CFR engine (600 rpm). Table 4 provides an overview of key operating conditions of the developed Supercharged Octane Number test method and boosted modern engine test from Szybist et al. [21]. Figure 8 shows a correlation between previously discussed KLCA50 data from Szybist et al. in Figures 4 and 5 and the newly introduced SON ratings at 1.5 bar intake pressure on the CFR engine. The trendline indicates an advanced KLCA50 for an increased SON, which is the desired trend. To reiterate, KLCA50 and RON failed to have any correlation in Figure 4. The SON rating of PRF100 overestimated its knock-limited combustion phasing in a boosted GDI engine. As discussed previously, PRFs reduced their compression ratio more rapidly than any of the other fuels in Figure 6. TSF96.9 outperformed its SON rating, suggesting that its knock resistance in a boosted GDI engine is even higher than its SON rating. Neither RON, nor OI, nor SON were able to capture the unexpectedly high knock resistance of TSF96.9. The overall coefficient of determination of SON is slightly worse than the KLCA50 comparison to OI. That is expected to some extent since OI uses the K-factor to iterate anywhere within the beyond RON space, while the SON was tested at one specific pressure-temperature trajectory. A similar approach to OI, just with new interpolation brackets of SON and RON is therefore introduced in the following section.

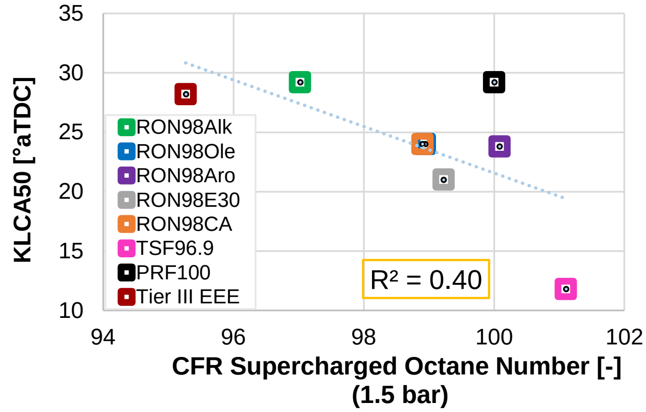

Figure 8. KLCA50 correlation to Supercharged Octane Number at 1.5 bar intake pressure conditions. KLCA50 data from Szybist et al. at 2000 rpm, 40 °C, 1.5 bar intake pressure [21]

There is one major difference between the developed SON test method and the knock-limited testing capabilities of modern research engines. The CFR engine can utilize its unique variable compression ratio system to adjust for knock intensity while most other engines vary the spark timing to adjust knock intensity. To align the testing methodology on both engines, a second SON test method with variable spark timing and constant compression ratio at otherwise equal testing conditions was investigated on the CFR engine. For this, the knock-limited spark advance (KLSA) of sample fuels was interpolated relative to that of PRFs. However, this can only be applied to fuels with similar knock resistance since otherwise, significant ranges of combustion phasing would be required. The previously discussed compression ratio (CR)-based SON had a similar combustion phasing due to a fixed spark timing between fuels, which allowed testing of fuels with a wider range of knock resistance. Furthermore, the KLSA-based SON determination requires changes in combustion phasing depending on the knock resistance of the fuel which subsequently results in differences in the indicated mean effective pressure (IMEP) between fuels. The shift in combustion phasing between fuels is a major disadvantage of the KLSA-based SON over the CR-based SON test methodology, which used a constant spark timing and therefore similar IMEPs.

Figure 9 shows a comparison of the previously discussed CR-based SON to the newly introduced KLSA-based SON. Both were tested at 1.5 bar intake pressure, 52 °C intake air temperature, and 600 rpm. The KLSA-based SON had a fixed compression ratio of 6.4:1, while the CR-based SON varied in compression ratio between 5.5 and 6.4:1, Figure 6. Overall, the CR-based SON and the KLSA-based SON align well and the linear trendline has an excellent correlation factor when excluding PRF100. When including PRF100, the coefficient of determination drops noticeably. PRF100 is the outlier in this data set that falls off of the trendline, meaning that it experienced the greatest impact from a change in combustion phasing. Paraffinic fuels are known for their low-temperature chemistry, which is greatly impacted by the available time for the reactions [13, 14]. Furthermore, since PRF100 is the reference fuel for interpolation of the SON of all sample fuels, each fuel experienced a significant shift in KLSA-based SON. This is visualized by the difference in extrapolation requirement in Figure 9. The CR-based SON method only required slight extrapolation beyond 100 for TSF96.9 and RON98Aro, while for the KLSA-based SON, most of the sample fuels required a significant extrapolation beyond 100. This is another disadvantage for the KLSA-based SON over the CR-based variant. It is positively noted, that TSF96.9 falls close to the trendline for the first time. Therefore, both SON methods work similarly well for highly aromatic fuels.

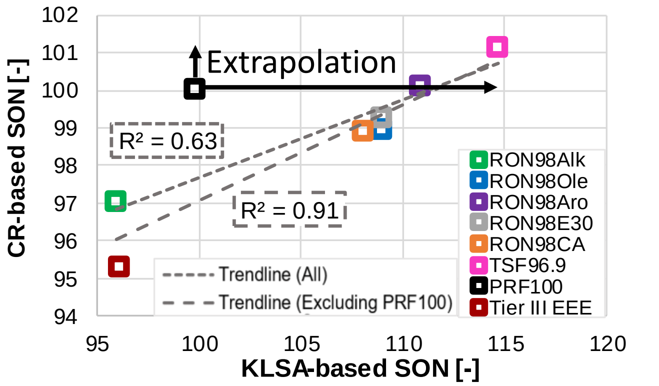

Figure 9. Compression ratio-based SON correlation to a knock-limited spark timing-based SON. Both methods were tested at 1.5 bar intake pressure, 52 °C intake temperature, and 600 rpm.

Supercharged Octane Index

Figure 5 showed that OI breaks down for highly aromatic fuels such as TSF96.9 when tested at high intake pressures. This can be caused by the extrapolation far outside of the RON-MON boundaries. The newly developed SON method can be used to create a new OI_S that follows a similar concept to the standard OI. Equation 2 shows the new formulation of OI_S using SON and RON as interpolation boundaries. A new K_S factor was introduced as an interpolation factor between SON and RON. For RON operation, K_S is identical to K with a defined value of 0. For SON conditions, K_S equals -1. Besides RON, K_S and K are not at an identical scale since the RON-MON sensitivity differs from the SON-RON sensitivity. Figure 10 depicts the K-value distribution as well as the applicable ranges for OI_S and OI. All cases from RON to beyond MON conditions at high temperatures are covered by the conventional OI. Cases with elevated intake pressures in the beyond RON region use the newly introduced OI_S.

$$OI_S = RON - K_S * (SON - RON) \quad (2)$$

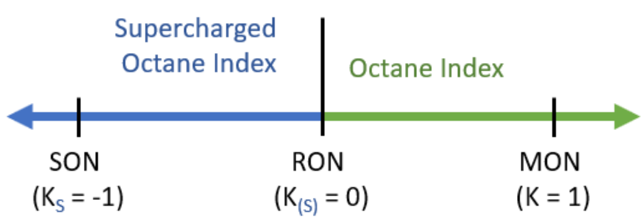

Figure 10. Schematic of OI_S and conventional OI applicability relative to SON, RON, and MON.

Figure 11 shows the correlation between the previously discussed KLCA50 data from a boosted GDI engine operation from Szybist to the newly introduced OI_S. The new K_S factor was optimized for the best correlation. Both the CR-based and the KLSA-based SON ratings were used separately for the OI_S calculations and are marked with different symbols and two different trendlines. Both OI_S correlations had similar coefficients of determination and showed significant improvements over the KLCA50 correlation to the conventional OI in Figure 5. However, the KLSA-based OI_S has a noticeable offset from the CR-based OI_S which is attributed to the large SON offset from Figure 9. While a large extrapolation beyond 100 was required for the KLSA-based OI_S, an equally good correlation to the CR-based OI_S was found. Both OI_S trendlines also required an identical K_S factor of -2.25. A negative K_S factor was expected since the engine was operated in the beyond RON range. However, a K_S lower than -1 still required an extrapolation beyond SON conditions suggesting that yet higher intake pressures might be required for the SON test method. Nonetheless, the OI_S proved superior over the conventional OI when comparing the KLCA50 data from a boosted GDI engine. The CR-based OI_S also mostly captured the knock resistance of TSF96.9.

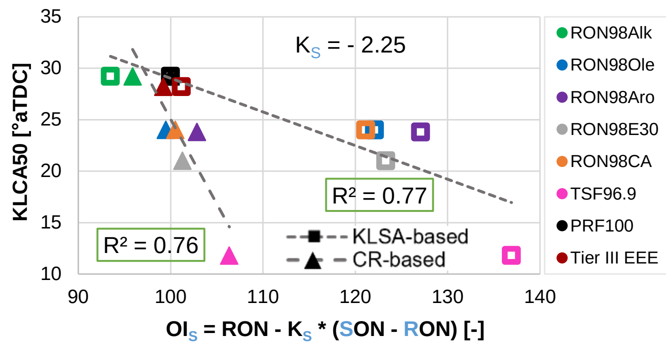

Figure 11. Correlation of the newly introduced OI_S for the CR-based and the KSLA-based SON to KLCA50 data operated at 2000 rpm, 40 °C, 1.5 bar intake pressure by Szybist et al. [21].

Open Challenges of the SON Method

This is the first experimental data of a Supercharged Octane Number test performed on a CFR engine that was designed for RON operation. The SON results were incorporated into a newly developed OI_S methodology. It is noted that the authors do not claim to publish a finalized SON test method, but rather show the concept of the framework and developments made so far. The authors are aware of certain limitations and required future work. The shift away from the standardized knockmeter system to a cylinder pressure transducer-based knock intensity threshold requires validation. Furthermore, a repeat test with the D1 Detonation Pickup could simplify the changeover procedure from RON to SON testing. While the authors previously published work on shifting lambda away from peak knock intensity to stoichiometric operation, the impacts on knock intensity at elevated intake pressures need to be investigated [17, 18]. The new SON method also does not have a functional Fit for Use test, which can be challenging to implement due to the vast difference in knock behavior between PRF and TSF at boosted conditions. The authors performed Fit for Use tests under standard RON operation with all engine upgrades installed, which the engine passed without any temperature tuning. Establishing a Fit for Use procedure might require an inter-laboratory study, which would also need to establish the repeatability and reproducibility values for the SON method.

This research revealed that higher intake pressure beyond 1.5 bar in the CFR SON test method might be useful to further improve the correlation to boosted GDI engines. A target intake pressure needs to be selected, tested, and validated against knock-limited boosted engine operation. Furthermore, the pressure-temperature trajectory of the newly developed SON test needs to be calculated and compared to those of RON and MON. A closer analysis of pressure-temperature conditions can also help to investigate the large offset between the CR-based and the KLSA-based SON methods since low-temperature chemistry is suspected. Nonetheless, the proposed SON methods along with the introduced OI_S calculations improved the correlations to knock-limited engine operation at beyond RON conditions, which represents the knock-limited operation of boosted engines.

Summary and Conclusions

This work developed a SON test method and implemented the required upgrades on a CFR engine. Furthermore, a new OI_S was introduced, which uses the new SON. This resulted in the following conclusions:

- The pressure-temperature trajectories of RON and MON do not adequately bracket the knock-limited operation of modern boosted engines in the beyond RON region, which requires extrapolation of the OI outside of its boundaries.
- The selected fuel matrix for this study was intentionally aligned with available data sets of knock-limited boosted gasoline direct injection engine operation to allow for an evaluation of newly introduced octane methods.
- The CFR engine was upgraded with modern combustion research instrumentation and a compressed air intake system while retaining the standard carburetor.
- Two versions of a SON test method were evaluated with advantages of the CR-based SON over the KLSA-based SON.
- The CR-based SON significantly improved the correlation to knock-limited combustion phasing data from a boosted gasoline direct injection engine over standard RON.
- A new Supercharged OI was introduced, which used the SON and RON as interpolation boundaries and significantly improved the correlation to the knock-limited operation of a boosted gasoline direct injection engine over the conventional OI.
- Current challenges of the newly developed SON method are presented and discussed to provide an overview of future work items.

References

1. Department of Transportation, National Highway Traffic Safety Administration, “Corporate Average Fuel Economy Standards for Model Years 2024-2026 Passenger Cars and Light Trucks”, 49 CFR Parts 523, 531, 533, 536, and 537, 2022.
2. European Parliament, “Setting CO2 emissions performance standards for new passenger cars and for new light commercial vehicles, and repealing regulations (EC) No 443/2009 and (EU) No 510/2011”, Regulation (EU) 2019-631, 2019.
3. Yates, A., Swarts, A., and Viljoen, C., "Correlating Auto-Ignition Delays And Knock-Limited Spark-Advance Data For Different Types Of Fuel," SAE Technical Paper 2005-01-2083, 2005, https://doi.org/10.4271/2005-01-2083.
4. ASTM D2699-22, “Standard Test Method for Research Octane Number of Spark-Ignition Engine Fuel,” ASTM International, West Conshohocken, PA, 2022, doi: 10.1520/D2699-22.

5. ASTM D2700-22a, “Standard Test Method for Motor Octane Number of Spark-Ignition Engine Fuel,” ASTM International, West Conshohocken, PA, 2016, doi: 10.1520/D2700-22a
6. Pulpeiro Gonzalez, J., Waqas, M., Kolodziej, C., DelVescovo, D. et al., "Improvements to a CFR Engine Three Pressure Analysis GT-Power Model for HCCI and SI Conditions," SAE Technical Paper 2019-32-0608, 2020.
7. Bartholomew, E., "NEW KNOCK-TESTING METHODS NEEDED TO MATCH ENGINE AND FUEL PROGRESS," SAE Technical Paper 610200, 1961, https://doi.org/10.4271/610200.
8. Trimble, H., “Report on the Development of the Antiknock Scale Above 100 Octane Number (1930-1958)”, ATM International Committee D02 on Petroleum Products and Lubricants, 1978.
9. Swarts, A., Yates, A., Viljoen, C., and Coetzer, R., "A Further Study of Inconsistencies between Autoignition and Knock Intensity in the CFR Octane Rating Engine," SAE Technical Paper 2005-01-2081, 2005, https://doi.org/10.4271/2005-01-2081.
10. Mittal, V., “A study of the Physics and Chemistry of Knock in Modern I Engines and Their Relationship to the Octane Tests”, Dissertation Massachusetts Institute of Technology, 2009.
11. Mittal, V. and Heywood, J., "The Shift in Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines Over the Last 70 Years," SAE Int. J. Engines 2(2):1-10, 2010, doi:10.4271/2009-01-2622.
12. Kalghatgi, G., "Fuel Anti-Knock Quality- Part II. Vehicle Studies - How Relevant is Motor Octane Number (MON) in Modern Engines?," SAE Technical Paper 2001-01-3585, 2001, doi:10.4271/2001-01-3585.
13. Waqas, M., Cheng, S., Goldsborough, S., et a., “An experimental and numerical investigation to characterize the low-temperature heat release in stoichiometric and lean combustion”, Proceedings of the Combustion Institute, Volume 38, Issue 4, 2021. https://doi.org/10.1016/j.proci.2020.07.146.
14. DelVescovo, D., Splitter, D., Szybist, J., et a., “Modeling pre-spark heat release and low temperature chemistry of iso-octane in a booste spark-ignition engine”, Combustion and Flame, Volume 212, Pages 39-52, 2020, https://doi.org/10.1016/j.combustflame.2019.10.009.
15. Mittal, V. and Heywood, J., "The Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines," SAE Technical Paper 2008-01-2414, 2008, doi:10.4271/2008-01-2414.
16. Salih, S. and DelVescovo, D., "Design and Validation of a GT Power Model of the CFR Engine towards the Development of a Boosted Octane Number," SAE Technical Paper 2018-01-0214, 2018, https://doi.org/10.4271/2018-01-0214.
17. Hoth, A., Pulpeiro Gonzalez, J., Kolodziej, C., and Rockstroh, T., "Effects of Lambda on Knocking Characteristics and RON Rating," SAE Int. J. Adv. & Curr. Prac. in Mobility 1(3):1188-1201, 2019, https://doi.org/10.4271/2019-01-0627.
18. Hoth, A., Kolodziej, C., “Effects of Knock Intensity Measurement Technique and Fuel Chemical Composition on the Research Octane Number (RON) of FACE Gasolines: Part 1 – Lambda and Knock Characterization”, Fuel, Volume 304, 2021, https://doi.org/10.1016/j.fuel.2021.120722.
19. Hoth, A., Kolodziej, C., Rockstroh, T., and Wallner, T., "Combustion Characteristics of PRF and TSF Ethanol Blends with RON 98 in an Instrumented CFR Engine," SAE Technical Paper 2018-01-1672, 2018, https://doi.org/10.4271/2018-01-1672.
20. Rockstroh, T., Kolodziej, C., Jespersen, M., Goldsborough, S. et al., "Insights into Engine Knock: Comparison of Knock Metrics across Ranges of Intake Temperature and Pressure in the CFR

Engine," *SAE Int. J. Fuels Lubr.* 11(4):545-561, 2018, https://doi.org/10.4271/2018-01-0210.

21. Szybist, J., Splitter, D., "Impact of Engine Pressure-Temperature Trajectory on Autoignition for Varying Fuel Properties", Applications in Energy and Combustion Science, Volumes 1-, 2020, https://doi.org/10.1016/j.jaecs.2020.100003.
22. Fouts L, Fioroni G, Christensen E, RatcliffMA, McCormick R, Zigler BT, et al. Prop- erties of Co-optima core research gasolines. National Renewable Energy Laboratory Technical Report NREL/TP-5400-71341, 2018.
23. Swarts, A., Anderson, G., and Wallace, J., "Comparing Knock between the CFR Engine and a Single Cylinder Research Engine," SAE Technical Paper 2019-01-2156, 2019, https://doi.org/10.4271/2019-01-2156.
24. Hauber, J., Huber, K., and Nell, R., "New GKI - Gasoline Knock Index for Rating of Fuel's Knock Resistance on an Upgraded CFR Test Engine," SAE Technical Paper 2018-01-1743, 2018, doi:10.4271/2018-01-1743.
25. Waqas, M., Hoth, A., Kolodziej, C., et al., "Detection of low temperature heat release (LTHR) in the standard Cooperative Fuel Research (CFR) engine in both SI and HCCI combustion modes", Fuel, Volume 256, 2019, 115745, https://doi.org/10.1016/j.fuel.2019.115745.

Contact Information

Alexander Hoth, ahoth@anl.gov, ahoth@mtu.edu

Christopher P. Kolodziej, ckolodziej@anl.gov

Acknowledgments

The authors would like to thank Timothy Rutter for his technical support in the laboratory. The authors are also thankful for the support of the group's section manager Doug Longman.

The submitted manuscript has been created in part by UChicago Argonne, LLC, Operator of Argonne National Laboratory ("Argonne") and Oak Ridge National Laboratory ("ORNL"). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357 and ORNL is a U.S. Department of Energy Office of Science laboratory managed by UT-Battelle under contract DE-AC05-00OR22725. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the DOE Public Access Plan. http://energy.gov/ downloads/doe-public-access-plan. This work is performed under the auspices of the Office of Energy Efficiency and Renewable Energy, Office of Vehicle Technology, U.S. Department of Energy, as part of the Co-Optimization of Fuels & Engines (Co-Optima) Program. Special thanks to the Vehicle Tech-nologies Office program managers Kevin Stork, Gurpreet Singh, Leo Breton, and Mike Weismiller, as well as the Bioenergy Technology Office Program manager Alicia Lindauer.

Abbreviations

AKI	Anti-Knock Index
CAD	Crank Angle Degree
CFR	Cooperative Fuel Research
CR	Compression Ratio
GDI	Gasoline Direct Injection
IMEP	Indicated Mean Effective Pressure
KLCA50	Knock-Limited combustion phasing for 50% mass fraction burned
KLSA	Knock-Limited Spark Advance
MAPO	Maximum Amplitude of Pressure Oscillations
MON	Motor Octane Number
NTC	Negative Temperature Coefficient
OI	Octane Index
OI_S	Supercharged Octane Index
PRF	Primary Reference Fuel
R^2	Coefficient of Determination
RON	Research Octane Number
SI	Spark Ignition
SON	Supercharged Octane Number
ST	Spark timing
TEL	Tetraethyl Lead
TSF	Toluene Standardization Fuel