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DEVELOPMENT OF ADVANCED COMPRESSION IGNITION (ACI) GASOLINE RATING METHODS ON A VARIABLE COMPRESSION RATIO CFR ENGINE

Final Report

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Development of Advanced Compression Ignition (ACI) Gasoline Rating Methods on a Variable Compression Ratio CFR Engine

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Executive Summary

Diesel is the conventional fuel of compression ignition engines, but advanced combustion research has demonstrated the potential for efficiency and emissions improvements of these engines with gasoline-like fuels. One barrier to adoption is the lack of a compression ignition rating method for gasoline-like fuels. This project explores the possibility of using the widely available CFR F1/F2 octane rating engine to rate gasolines for modern Advanced Compression Ignition (ACI) engines, such as light duty (LD) multi-mode (MM) and medium duty/heavy duty (MD/HD) ACI engines.

This work investigated four aspects to enhancing the CFR engine HCCI rating method. First, it was found that the standard CFR engine knock sensor, the D1 pickup, is sufficiently accurate to measure combustion phasing within the uncertainty of a modern piezoelectric cylinder pressure transducer, with the cetane rating pickup having slightly higher uncertainty. Second, after assessing and making engine modifications, the highest geometric compression ratio of the CFR engine was increased to 23.6:1 and an unshrouded intake valve was installed to maximize naturally aspirated cylinder pressure conditions in order to rate the compression ignition reactivity of up to 87 anti-knock index (AKI) gasolines at low-reactivity idle-like engine conditions. Third, the carburetor was replaced with a newly designed port fuel injection and the intake system was upgraded to

allow maximum intake air conditions up to 3.0 bara and 300 °C. Fourth, the standard torque absorption motor was upgraded to work with a variable frequency drive, allowing for up to 1,800 RPM engine test speeds.

The 23 test fuels ranged from a research octane number (RON) of 60 to 94. Ten of the test fuels were based on a commercial 87 AKI E10 gasoline, exchanging the ethanol with other biofuel blend stocks (isobutanol, prenol, isopentanol, diisobutylene, and n-butanol), using isooctane, diisobutylene, toluene, and n-heptane to hone in the target 87 AKI while varying their aromatic and olefinic content. Across the range of test conditions studied, higher aromatic (toluene) gasolines had the lowest compression ignition reactivity for their RON rating. Olefinic (diisobutylene) gasolines and the prenol-blended gasoline showed increased compression ignition reactivity with increasing intake air temperature relative to the other test fuels. Substituting ethanol with higher carbon-number alcohols led to increased compression ignition reactivity across some to all test conditions, depending on the alcohol. Testing these fuels on a single-cylinder heavy-duty gasoline compression ignition engine showed a strong correlation of fuel performance with their CFR engine-based compression ignition reactivity ratings.

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1. **Introduction**

Advanced Compression Ignition (ACI) engines represent a promising pathway for achieving high efficiency and low emissions in internal combustion engines. Among the various ACI methods, Homogeneous Charge Compression Ignition (HCCI) is attractive due to its ability to achieve near-zero NOx and particulate emissions while maintaining high thermal efficiency. However, HCCI faces challenges related to combustion control, particularly at low and high load conditions. Other ACI methods, such as Reactivity Controlled Compression Ignition (RCCI), Gasoline Compression Ignition (GCI), Partially Premixed Compression Ignition (PPCI), etc., have been explored to address these limitations, but each approach requires a nuanced understanding of fuel properties and combustion dynamics.

The widely available Cooperative Fuel Research (CFR) F1/F2 octane rating engine at Argonne National Laboratory has been adapted to investigate the compression ignition propensity of homogeneous charge mixtures. This adaptation leverages the CFR engine's variable compression ratio capabilities to simulate conditions relevant to ACI combustion. By modifying the CFR engine to operate under HCCI test conditions, autoignition characteristics of fuels across a wide range of thermodynamic and temporal conditions are evaluated in this work.

This study builds upon the historical significance and international utilization (>2,000 units) of the CFR engine, which has been fundamental for fuel characterization in spark-ignited engines, and extends its test capabilities to the domain of ACI engines. Modifications to the CFR engine include hardware upgrades such as increased compression ratio, electronic fuel injection, high-temperature intake and exhaust systems, and advanced data acquisition and control systems. These upgrades enable the engine to operate at higher intake pressures (up to 3.0 bara), intake temperatures (up to 300°C), and engine speeds (up to 1800 RPM), significantly expanding its capability to characterize fuels under ACI conditions.

Despite advancements in ACI engine technology, there remains a critical research gap in understanding autoignition behavior in ACI engines fueled with blends of varied aromatic and olefinic content. Additionally, key challenges include maintaining engine stability during low-load and cold-start conditions, as well as addressing high-load scenarios characterized by high pressure and low temperature.

To address these challenges, this study investigates the autoignition characteristics of 87 AKI E10 gasoline blended with alternative bio-derived blendstocks, including isobutanol, prenol, isopentanol, diisobutylene, and n-butanol. These blendstocks were selected for their potential to enhance fuel reactivity and compatibility with ACI combustion strategies, while still meeting the 87 AKI octane requirements for spark-ignition engines and abiding by the ASTM D4814 2.7 wt% maximum gasoline oxygen content limit. By quantifying the autoignition behavior of these blends under controlled HCCI conditions, this research aims to provide insights into fuel-engine interactions that are critical for optimizing ACI engine performance.

Additionally, the study seeks to develop correlations between CFR ACI fuel metrics and modern ACI engine performance, particularly for Medium-Duty/Heavy-Duty (MD/HD) combustion strategies. This effort aligns with the broader goals of the Co-Optimization of Fuels and Engines (Co-Optima) program, which aims to identify fuel properties and test methods that are most relevant for future engine technologies.

2. <u>Experimental Setup</u>

With the CFR engine as the base experimental platform for this work, numerous upgrades were added to extend the range of operating conditions and for modern engine data collection. Such upgrades were crucial to achieve the necessary in-cylinder conditions to conduct investigation of ACI engine regimes. Additionally, a Caterpillar single-cylinder heavy-duty engine was utilized for this work to evaluate fuel reactivity trends on a representative MD/HD engine platform.

2.1 Engines Specifications

The CFR engine was originally developed in the early 1930s as a standard engine to evaluate knocking propensity of fuels at standardized operating conditions. It continues to serve this purpose today with ASTM standard methods for quantifying the research octane number (RON, ASTM D2699) and motor octane number (MON, ASTM D2700). As mentioned, the CFR used in this work received many upgrades to extend its capabilities, but it maintains its original internal geometry and full compliance with ASTM standards for RON and MON testing. Key engine parameters can be found in Table 1 with new/upgraded capabilities shown in parentheses. New and upgraded CFR engine capabilities are detailed in Sections 2.2-2.4.

Besides the updated CFR engine, which was the primary research tool in this project, a heavy-duty GCI Engine was utilized to study the impact of engine architecture on fuel reactivity trends measured by the CFR engine. These experiments were conducted using a single-cylinder heavy-duty diesel engine based on a modified Single Cylinder Oil Testing Engine (SCOTE) from Caterpillar. The SCOTE engine specifications can be found in Table 2. The engine was outfitted with a high-pressure common rail injection system (to replace its original mechanical injection system) and the cylinder head was modified to install research instrumentation. This engine will be referred to as the HD-SCE (Heavy-Duty Single Cylinder Engine) in the remainder of this report.

Table 1: Overview of CFR engine parameters

Parameter	**CFR Engine Original (New)**
Displacement	0.612 L
Cylinder Bore	8.255 cm
Stroke	11.43 cm
Compression Ratio	Continuously variable from 4.1 to 18:1 (23.6:1)
Fuel System	Carbureted (port injected) with four fuel bowls
Intake Valve	One shrouded non-rotating valve (unshrouded)
Exhaust Valve	One unshrouded rotating valve
Valve overlap	5 CAD
Piston Geometry	Flat top
Spark Plug	Side-mounted

Table 2: Overview of HD-SCE engine parameters

Parameter	**Value**
Displacement	2.44 L
Cylinder Bore	13.72 cm
Stroke	16.51 cm
Compression Ratio	15.3:1
Fuel System	Common Rail Direct Injection

2.2 CFR Engine Upgrades, Phase 1

The range of variable compression ratios for the CFR engine was extended from its original design with a maximum of 18.4:1 to 23.6:1. The compression ratio is adjustable by raising/lowering the cylinder head thereby varying the clearance volume while maintaining a constant displaced volume or stroke (Fig. 1). In the original design, moving parts (such as the worm shaft housing and water outlet fitting) in the cylinder head assembly collided, preventing further increase in compression ratio. Therefore, a design study was conducted to modify the engine assembly to accordingly increase the compression ratio. As a result of the new design, the cylinder head can travel to a point at which there is a minimum of 1mm clearance between the top of the piston and the bottom of the exhaust valve, maintaining appropriate clearances for engine operation. However, it is important to note that in spite of these design changes to the adjustable cylinder head assembly, the interior of the combustion chamber was unchanged, meaning that the engine remains compliant with ASTM standards for RON and MON testing.

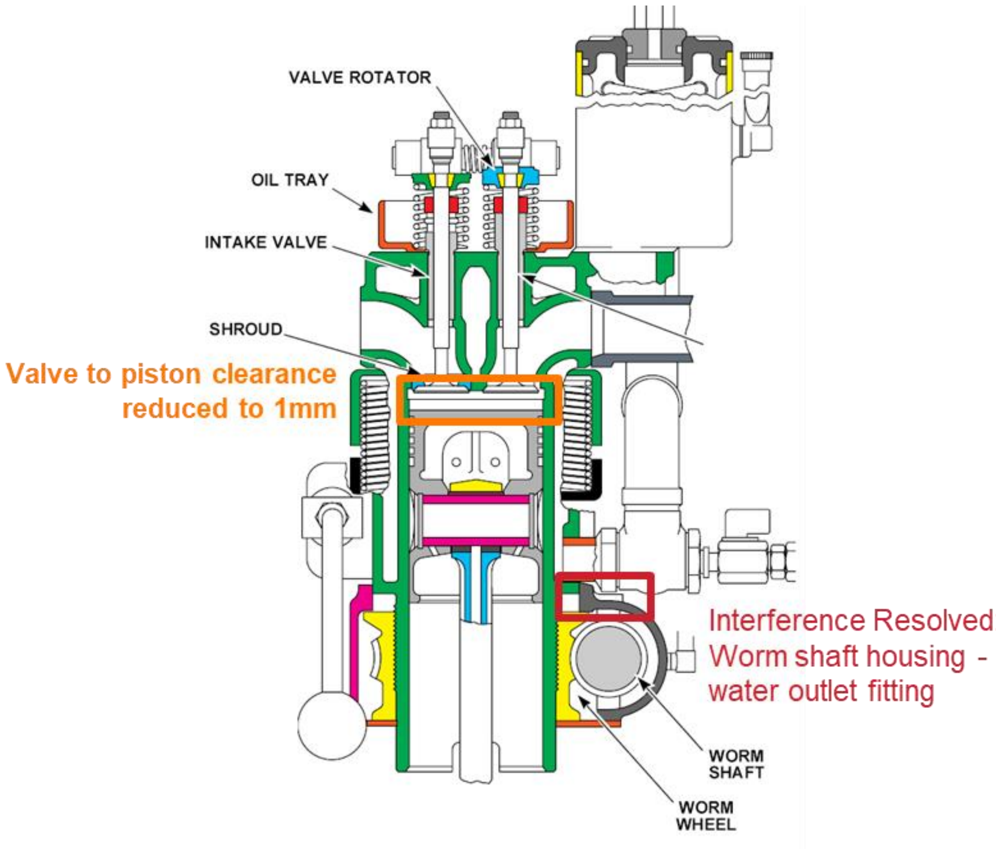
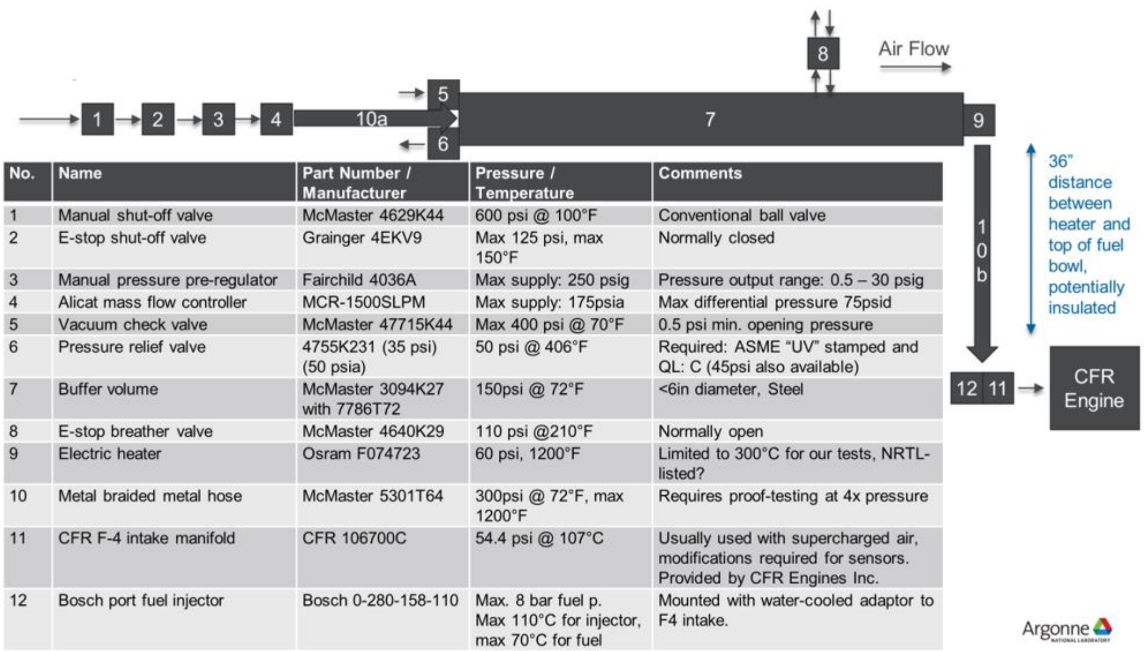


Figure 1: Schematic of key design modifications to the CFR engine to increase the range of variable compression ratios from 18.4:1 (original) to 23.6:1 (modified).

2.2 CFR Engine Upgrades, Phase 2

The engine intake system was modified from its original carbureted, naturally aspirated configuration to accommodate boosted intake pressures and elevated intake temperatures. To evaluate fuels for ACI engines, it is critical to explore an extended range of intake conditions to evaluate the influence on fuel reactivity and subsequent combustion.

Figure 2 shows a schematic of the intake system and a table to identify components. To achieve boost pressures up to 3 bara the intake air system was connected to the facility oil-free air compressor (Atlas Copco ZT75), a series of safety valves, a pressure regulator, and a mass flow controller control the air flow to the engine. A buffer volume (Item 7, Fig. 2) was included to dampen pressure pulsations from the engine and flexible braided stainless-steel hoses (Item 10, Fig. 2) isolate the solid tubing from the engine vibrations. A flow-through electric heater (Item 9, Fig. 2) preheats the intake air to the desired setpoint. Because of the increased intake pressure, a port fuel injection system (Item 12, Fig. 2) replaced the carburetor for consistent and controllable fuel delivery to the engine.



No.	Name	Part Number / Manufacturer	Pressure / Temperature	Comments
1	Manual shut-off valve	McMaster 4629K44	600 psi @ 100°F	Conventional ball valve
2	E-stop shut-off valve	Grainger 4EKV9	Max 125 psi, max 150°F	Normally closed
3	Manual pressure pre-regulator	Fairchild 4036A	Max supply: 250 psig	Pressure output range: 0.5 – 30 psig
4	Alicat mass flow controller	MCR-1500SLPM	Max supply: 175psia	Max differential pressure 75psid
5	Vacuum check valve	McMaster 47715K44	Max 400 psi @ 70°F	0.5 psi min. opening pressure
6	Pressure relief valve	4755K231 (35 psi) (50 psia)	50 psi @ 406°F	Required: ASME "UV" stamped and QL: C (45psi also available)
7	Buffer volume	McMaster 3094K27 with 7786T72	150psi @ 72°F	<6in diameter, Steel
8	E-stop breather valve	McMaster 4640K29	110 psi @210°F	Normally open
9	Electric heater	Osram F074723	60 psi, 1200°F	Limited to 300°C for our tests, NRTL-listed?
10	Metal braided metal hose	McMaster 5301T64	300psi @ 72°F, max 1200°F	Requires proof-testing at 4x pressure
11	CFR F-4 intake manifold	CFR 106700C	54.4 psi @ 107°C	Usually used with supercharged air, modifications required for sensors. Provided by CFR Engines Inc.
12	Bosch port fuel injector	Bosch 0-280-158-110	Max. 8 bar fuel p. Max 110°C for injector, max 70°C for fuel	Mounted with water-cooled adaptor to F4 intake.

Figure 2: Schematic and list of components in the modified intake system.

Additional details of the port fuel injection system are in Fig. 3. Notably, the four fuel canisters remain from the original CFR engine configuration to enable easy switching between test fuels and primary reference fuels. A Coriolis flow meter measures the fuel flow rate to a Bosch common rail and port fuel injector. Provisions are included to purge the fuel system with air.

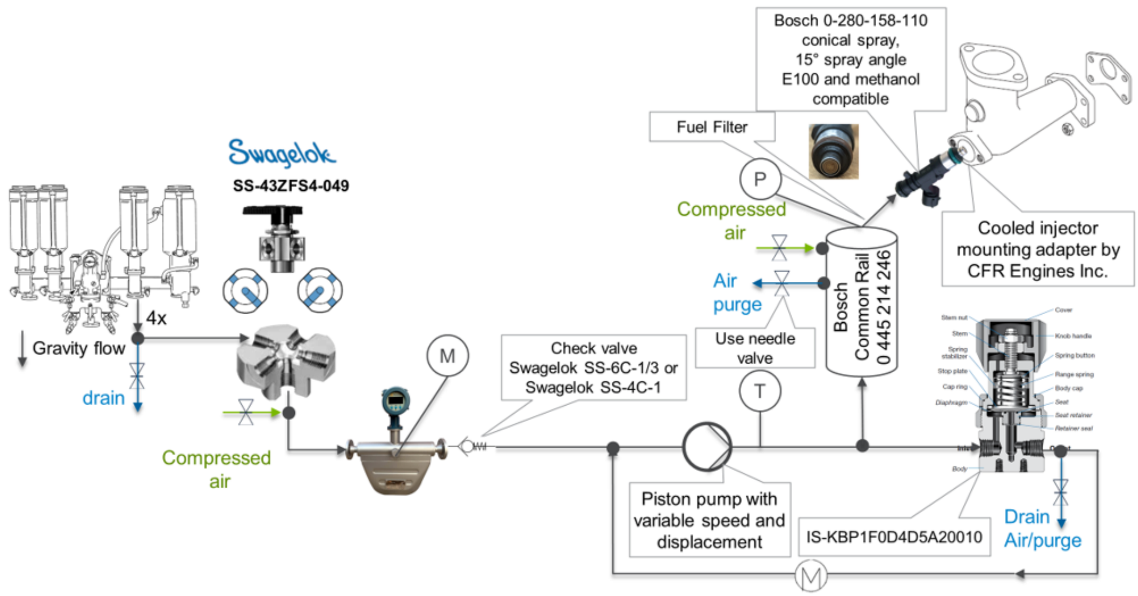


Figure 3: Schematic of the port fuel injection system.

2.3 CFR Engine Upgrade, Phase 3

Lastly, the data acquisition and control system for the CFR engine was upgraded to be a modern engine test cell. Equipped to handle crank angle-resolved and time-resolved measurement while controlling engine setpoints like fuel injection and air flow, the data acquisition system provides a high degree of flexibility and data robustness. Additionally, the latest CFR engine system, CFR XCP, was installed for the most advanced features. As a final extension of capabilities, a variable frequency drive can modulate the synchronous AC motor to enable varying engine speeds from 600-1800 RPM.

2.4 Instrumentation

3. Methodology

In-cylinder conditions were measured by a high-speed piezoelectric pressure transducer in this study to quantify the compression ignition reactivity of each fuel. However, through testing in this project, it was found that the standard CFR engine knock sensor, the D1 pickup, is sufficiently accurate to measure combustion phasing, and thus autoignition fuel reactivity. Indeed, the method for evaluating fuel reactivity in this study, the critical compression ratio (defined in Sec. 3.1), varied only by ±0.03 compression ratio by using the D1 pickup instead of an in-cylinder pressure transducer. Although the D1 pickup was not utilized in the results presented in this final report, it should be noted that the critical compression ratio could be evaluated on any of the >2,000 CFR F1/F2 engines currently in service worldwide using their existing in-cylinder instrumentation.

The work conducted in this program can be broken into three parts. First, a wide range of fuel blends including oxygenates were tested in the CFR engine to evaluate fuel reactivity for ACI engines compared to the standard RON test. Second, the ACI reactivity of gasolines with like anti-knock indices (87 AKI) and biofuel oxygen content (2.7 wt%), but select bioblendstock replacements for ethanol and varying aromatic and olefinic composition were evaluated across a wide range of engine operating conditions. Finally, a subset of fuels from Part 2 were tested in a heavy-duty GCI engine to correlate measurements with the CFR engine ratings to a more realistic heavy-duty engine application.

3.1 Performance Parameters and Calculations

Throughout the project, a set of common performance parameters and test methods were used to quantify the reactivity of each fuel blend.

The standard measurements of knock resistance in gasoline, RON and MON, were utilized as a baseline in this work and to categorize different groups of fuels. The full methods for obtaining RON and MON measurements are described by ASTM D2699 and D2700, respectively. Table 3 shows the key operating conditions for each respective metric.

Table 3: Overview of conditions for RON and MON

Parameter	RON	MON
Engine Speed	600 RPM	900 RPM
Intake Air Temperature	52 ^{o}C	38 ^{o}C
Mixture Air Temperature	Not controlled	149 ^{o}C
Spark Timing	13 ^{o}bTDC	Variable, depending on compression ratio
Lambda	Maximum Knock	Maximum Knock
Intake Pressure	Naturally aspirated, wide open throttle	Naturally aspirated, wide open throttle
Compression Ratio	Based on octane level and barometric pressure	Based on octane level and barometric pressure

Resulting from measurements of RON and MON, a fuel’s octane index (OI) can be derived. The commonly used gasoline anti-knock index (AKI) is defined by Eq. 1, when K is equal to 0.5.

$$Octane\ Index\ (OI) = RON - K * (RON - MON) \qquad \text{Eq. 1}$$

Critical Compression Ratio was then evaluated as a metric for ACI engines, also known as HCCI Critical CR in this work. The critical compression ratio was determined by gradually raising the compression ratio until a set combustion phasing is achieved.

Lastly, an assortment of standard engine testing metrics derived from in-cylinder pressure transducer measurements are reported in this work. The key metric used for identifying the critical compression ratio of the fuels under different test conditions was the crank angle degree of 50% fuel mass burned (CA50) (Fig. 4). Additionally, maximum pressure rise rate, ignition delay, standard deviation of CA50, standard deviation of combustion duration, standard deviation of peak pressure, and combustion efficiency are exemplified in Fig. 4.

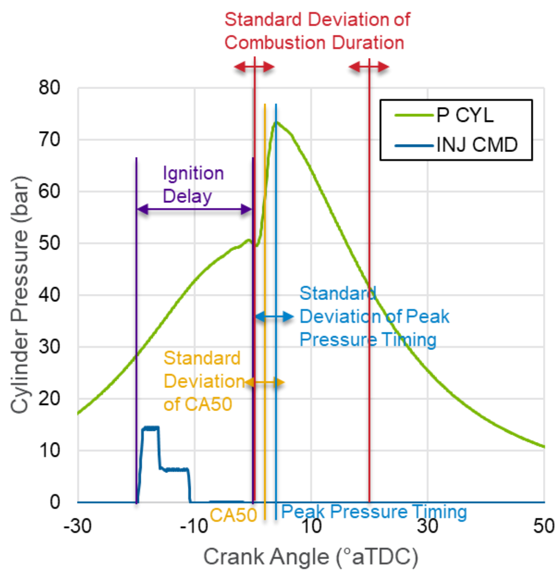


Figure 4: Standard engine testing metrics example.

3.1 Experiments, Phase 1

In Phase 1 of the experiments, fuels ranging from approximately 60 to 90 AKI were tested at a low intake pressure (1.0 bara), low intake temperature (45 °C) and medium speed (900 RPM) engine operating condition. The wide survey of fuels yielded comprehensive results to broadly compare fuel reactivity under compression ignition conditions to conventional spark-ignition knocking propensity (e.g., RON, MON, and AKI). Engine operating conditions and fuels tested can be found in Tables 4 and 5, respectively.

Table 4: Engine Operating conditions for Experiments, Phase 1

Lambda	3
Intake Mixture Temperature	45°C
Intake Pressure	1.0 bara
Engine Speed	900 RPM
CA50	3° aTDC
Compression Ratio	Adjusted to desired CA50
Load	~3 bar IMEP (nominal)

Table 5: Fuels tested in experiments, Phase 1

Fuel	RON	AKI
P66 RON60	59	58
P66 RON60 + iButA25	78	76
P66 RON60 + iButA51.2	94	90
P66 RON60 + E36.6	93	88
P66 RON70	71	70
P66 RON80	80	78
P66 RON91	91	87
MBOB-E9.8	89	87
MBOB-iButA15.5	89	87
MBOB-nButA15.4-iso20	90	87
MBOB-Prenol16.7	90	87
MBOB-iPentA18.4-iso15	89	87
MBOB-DIIB-iButA15.5-Hep5	90	87
MBOB-DIIB-nButA15.4	90	87
MBOB-DIIB-Prenol16.7-Hep3	91	87
MBOB-DIIB-iPentA18.4	90	87

*See nomenclature section for explanation of fuel abbreviations

3.2. Experiments, Phase 2

The experiments in the second phase focused on testing a down-selected number of fuels for a more controlled evaluation of the effect of oxygenated blendstocks (ethanol, isobutanol, isopentanol, and prenol) on compression ignition reactivity at a constant 87 AKI across a wide range of engine operating conditions. The fuel blends were carefully designed such that AKI was constant at around 87 AKI, once the target 2.7 wt% oxygenate level was obtained, by decreasing or increasing the AKI with primary reference fuels, n-heptane and iso-octane, respectively. Furthermore, diisobutylene and toluene were used to evaluate the impact of gasoline BOB olefinic or aromatic content, respectively. The fuels utilized in Experiments, Phase 2 are listed in Table 6, some of which were also tested in Experiments, Phase 1.

Table 6: Fuels Tested in Experiments, Phase 2

Fuel	Matrix inclusion criteria
MBOB-E9.8	Baseline
MBOB-iPentA18.4-isO15	Comparison of alcohols; low aromatic; low olefin
MBOB-Prenol16.7	Comparison of alcohols; low aromatic; low olefin
MBOB-iButA15.5	Comparison of alcohols; low aromatic; low olefin
MBOB-DIIB-iButA15.5-Hep5	Low aromatic; high olefin

MBOB-TOL-iButA16.2-Hep7	High aromatic; low olefin

The engine operating test matrix covered a wide range of operating conditions for each fuel by varying speed, intake air temperature, and intake pressure. The engine operating test matrix is tabulated in Table 7 and illustrated visually by Fig. 5. Select conditions also evaluated the fuel sensitivity to lambda by additionally evaluating lambda=4 as indicated by Fig. 5.

Table 7: Engine Operating conditions for Experiments, Phase 2; Swept parameters are shown in parentheses

Lambda	3 (4)
Intake Air Temperature	(50) 100 (150, 200)°C
Intake Pressure	1.0 (1.25, 1.5, 2.0) bara
Engine Speed	600 (1200, 1800) RPM
CA50	3° aTDC
Compression Ratio	Adjusted to rate fuel reactivity
Load	Variable (1.6-8.1 bar IMEP)

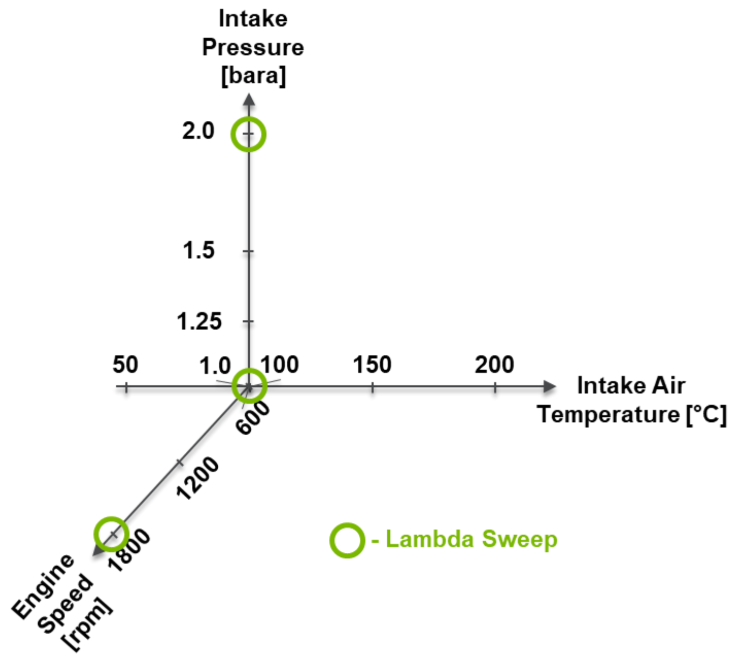


Figure 5: Engine test matrix for Experiments, Phase 2.

3.3 Experiments, Phase 3

Experiments conducted in Phase 3 evaluated the same fuels from Phase 2 (Table 8) on a GCI engine platform (HD-SCE, described in Sec. 2.1) to evaluate the impact of engine platform and fuel stratification on compression ignition reactivity.

For comparison to the CFR engine tests in Phase 2, similar operating conditions were tested in the HD-SCE. In particular, 1) a low-speed idle case, 2) a medium speed idle, and 3) a temperature sensitivity case were considered for comparison to the CFR engine results.

Table 8: Heavy-duty single-cylinder engine (HD-SCE) operating conditions for Experiments, Phase 3

Condition	**Low-Speed Idle**	**Medium-Speed Idle**	**Temperature Sensitivity**
Intake Air Temperature	60°C	60°C	100°C
Intake Pressure	1.0 bara	1.0 bara	1.0 bara
Engine Speed	600 RPM	1200 RPM	1200 RPM
Load	3 bar IMEP	3 bar IMEP	3 bar IMEP

4. <u>Results</u>

4.1 Results, Phase 1

The purpose of the phase 1 of experimentation was to investigate a large set of fuels in a compression ignition operation mode to compare the autoignition reactivity with traditional knock rating metrics (RON, MON, AKI). Therefore, the first tests were to measure traditional knock rating metrics with all fuels. Figure 6 shows the RON, MON, AKI, and sensitivity of each fuel. Figure 6a shows a subset of the fuel which is of similar AKI (~87), achieved by blending a variety of oxygenates and PRFs with a baseline gasoline (MBOB). Figure #b shows a subset of fuels with a wider range of knocking propensity.

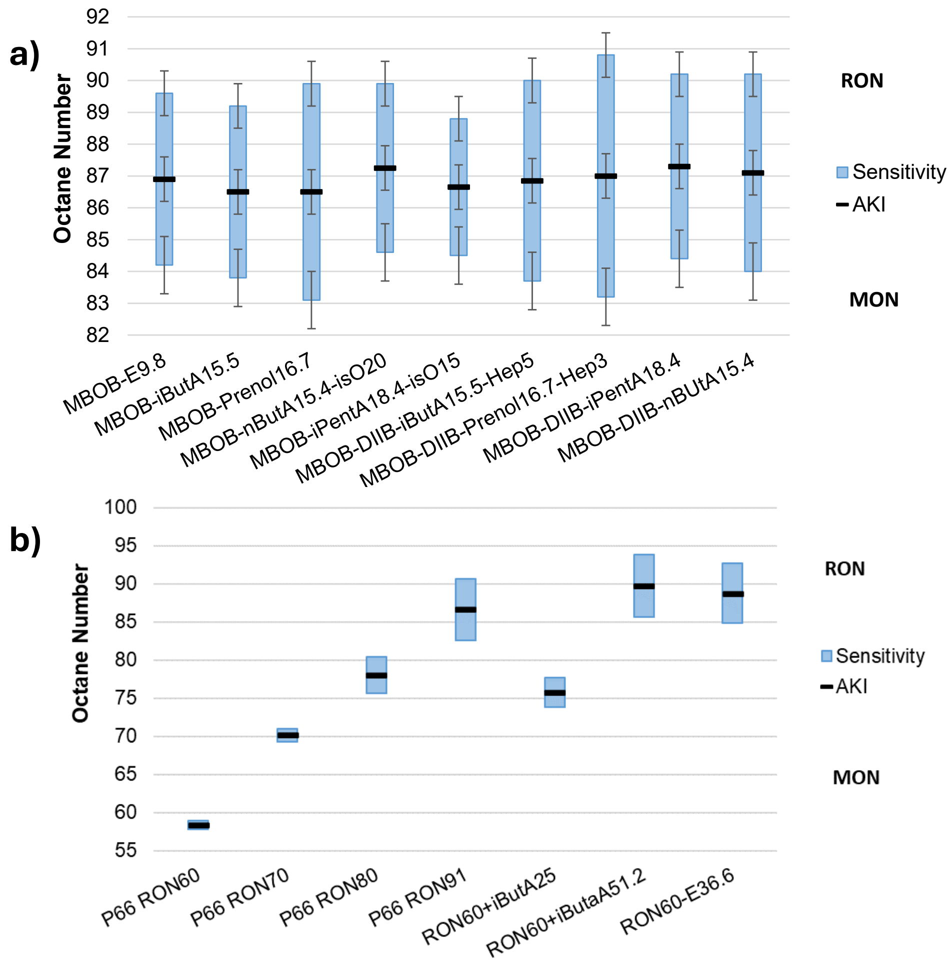


Figure 6: Knock rating metrics of fuels tested for Phase 1. a) shows a subset of fuels of similar AKI (~87), b) shows a subset of fuels broader range of knocking propensity

Next, the Critical Compression ratio was evaluated for each fuel and plotted against RON. A linear correlation would indicate that RON was a suitable metric for predicting autoignition reactivity of the fuels. Figure 7a shows that all fuels have a roughly linear correlation between Critical Compression Ratio and RON, however there are some significant deviations from the linear trend when looking closely at RON between 88 and 95, as shown in Fig. 7b. In particular, if knocking metrics were suitable for rating autoignition reactivity, the first subset of fuels (i.e., of similar AKI, RON, and MON) would all converge upon a similar Critical Compression Ratio. Figure 7b makes it obvious that fuels of similar RON do not follow a linear trend. Therefore a more nuanced approach is needed to unravel the significance of fuel properties and chemistry to autoignition reactivity. For instance, fuel blends with iso-pentanol and n-butanol required a lower Critical Compression Ratio (meaning would be easier to autoignite) than blends with ethanol and iso-butanol at a fixed AKI.

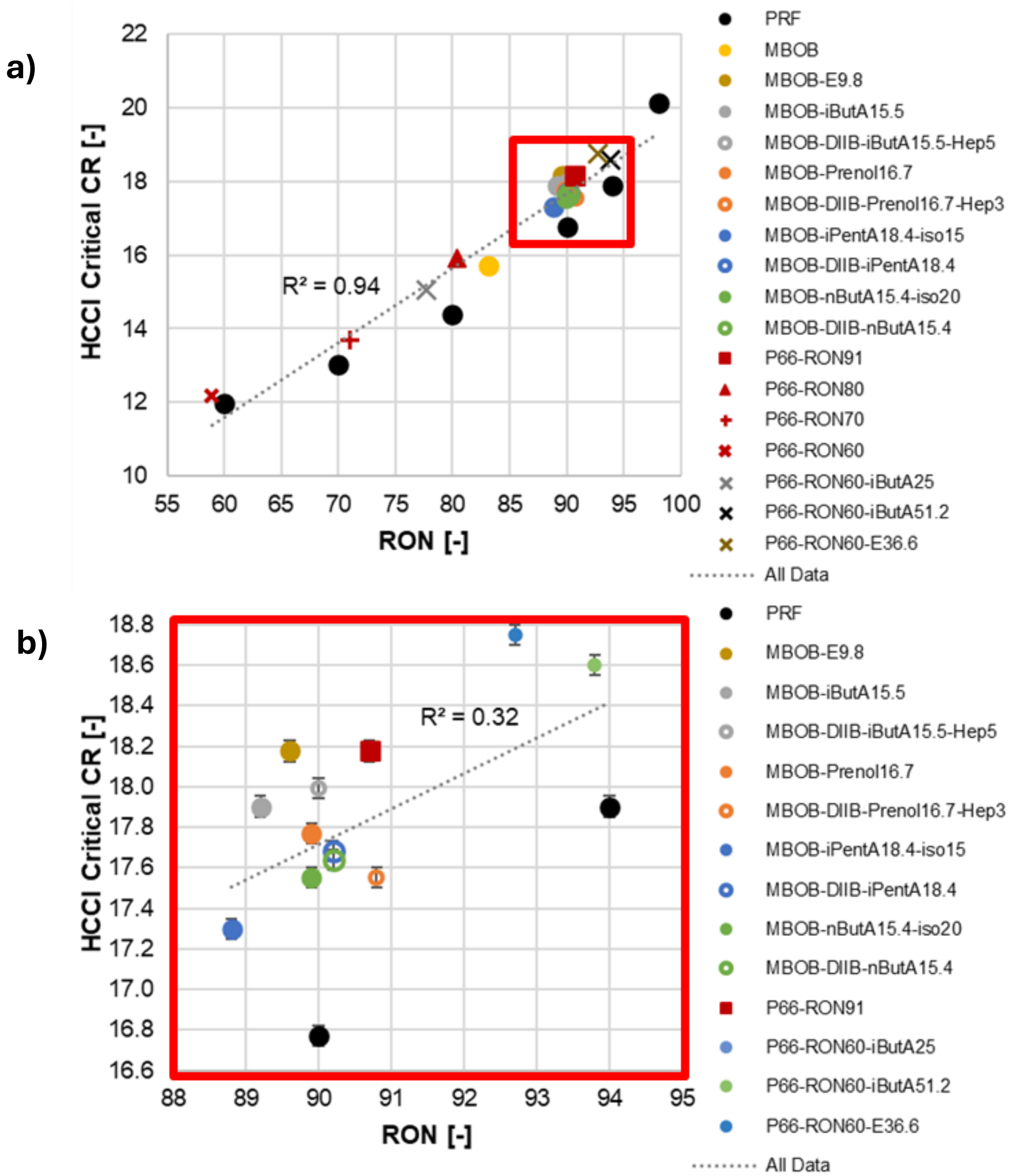


Figure 7: Correlation of RON with Critical Compression Ratio for Phase 1 experimentation. a) Broad trend over the entire dataset shows a roughly linear correlation, b) closer examination shows that there is significant deviation from the linear correlation as a result of fuel chemistry differences.

Coupled to an increase in Critical Compression Ratio is an increase in maximum pressure rise rate, as shown in Fig. 8. As such, factors such combustion noise and engine structural integrity, and corresponding control strategies, must be considered for the adoption of fuels requiring high critical compression ratio (i.e., high autoignition resistance) in ACI engines. At these low intake pressure and temperature conditions, some of the higher octane level fuels produced cylinder maximum pressure rise rates exceeding 10-11 bar/CAD. A few of these high critical compression ratio fuels even required the CA50 to be delayed by as much as 0.5-1 CAD (3.5-4 °aTDC) to limit maximum pressure rise rate during testing at these particular engine operating conditions, including:

- MBOB-E9.8
- MBOB-iButA15.5
- MBOB-nButA15.4-iso20
- MBOB-iPentA18.4-iso15
- MBOB-DIIB-nButA15.4

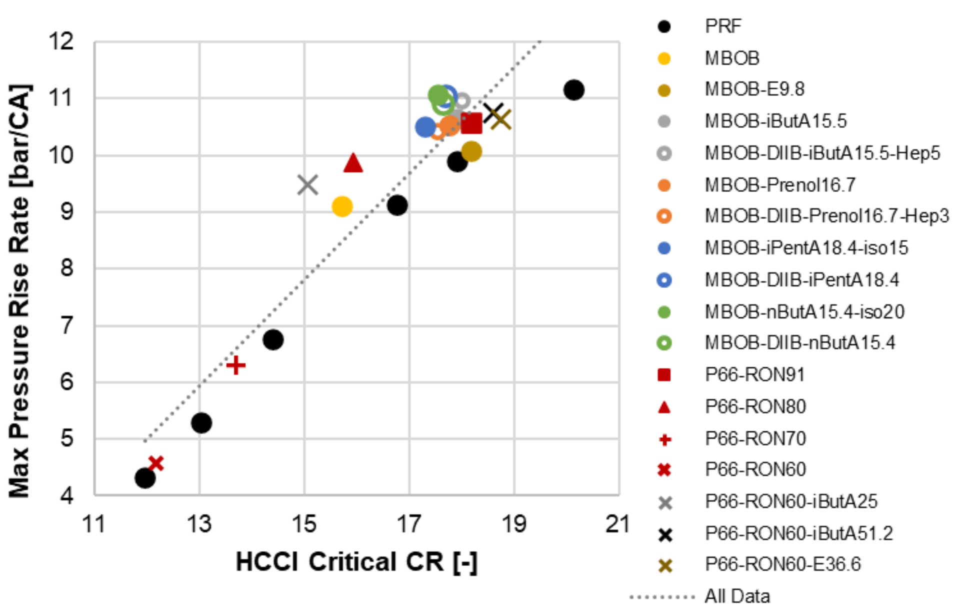


Figure 8: maximum pressure rise rates increase steeply with Critical Compression Ratio

It should be noted that Phase 1 results consider a single engine operating point, but clearly illustrate that there is a gap in characterizing autoignition reactivity by knocking metrics like RON, MON, or AKI. Phase 2 experiments were designed to probe more deeply into the impact of fuel chemistry on autoignition by performing a wider range of engine operating conditions and constraining fuels to be of similar knocking propensity.

4.2 Results, Phase 2

As mentioned in Sec. 3.2, the quantity of test fuels was reduced for Phase 2 experimentation to focus on the impact of olefinic and aromatic compounds across a wider range of engine operating conditions. As a baseline, standard RON, MON, AKI and octane sensitivity (the difference between RON and MON) is shown in Fig. 9. AKI was maintained constant for all test fuels. Additionally, the fuel bound oxygen was maintained constant for all test fuels.

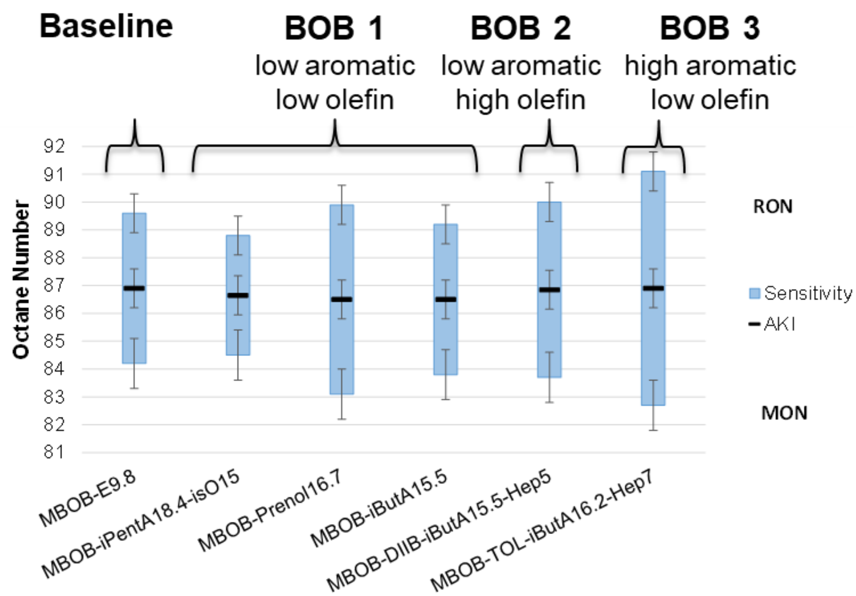


Figure 9: Knocking propensity metrics for Phase 2 test fuels.

A wide range of engine operating conditions were considered for Phase 2 experimentation, as discussed in Sec. 3.2. Varying engine speed, intake pressure, and intake temperature while holding lambda constant (except for a few operating points), results in a wide range of engine loads and in-cylinder pressure conditions. Table 9 shows the range of engine loads and pressure rise rates encountered throughout the course of testing. While the results of this study are focused on critical compression ratio, it is important to note that the test matrix permits variable engine loads and in-cylinder pressures.

Table 9: Range of engine load and in-cylinder pressure conditions across Phase 2 experiments

Parameter	$IMEP_g$ [bar]	Indicated Power [kW]	Max Pressure Rise Rate [bar/°CA]
Max	8.1	2.7	12.4

Min	1.6	0.5	3.6

4.2.1 Effect of intake temperature

As expected, preheating the intake mixture decreased the amount of compression ratio required to ignite the fuel and reach the threshold CA50, as shown in Fig. 10. Broadly speaking, all 87 AKI fuels encountered Critical Compression Ratios around 16.5-17.5 at the lowest intake temperature, reducing to around 13 at the highest temperature. Looking at individual fuels from left to right on the bar chart in Fig. 10, individual fuel trends can be interpreted. E10 and iBut15.5 exhibit similar behavior at all temperatures and consistently achieve critical compression ratios in the middle of the pack, at all intake temperatures. The yellow bar represents the fuel which is highly aromatic, iButA16.3-Tol-nHep7, and has the highest critical compression ratio at all temperatures; it is most resistant to autoignition. There is a trend reversal among the remaining three fuels, where the iPent18.4-IOct15 goes from being most reactive of all fuels at low temperatures, to similar reactivity as the 87 AKI E10 baseline fuel at high temperatures. Conversely, iButA15.5-DIIB-nHep5 and Prenol 16.7 initially had average reactivity at low temperature, but become the most reactive as temperature increases.

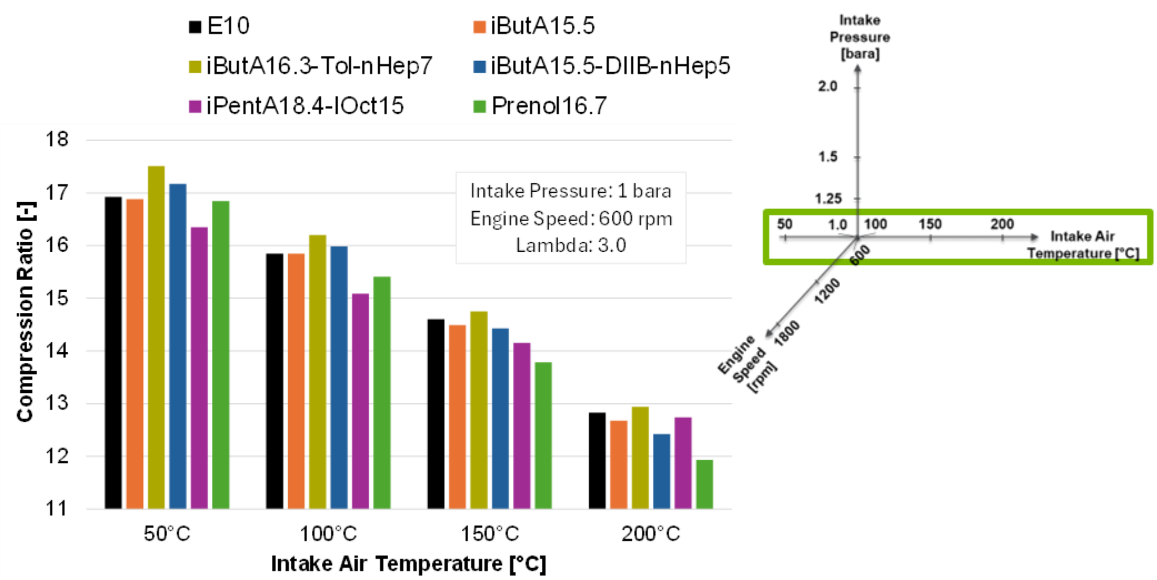


Figure 10: Effect of intake temperature on Critical Compression Ratio.

4.2.2 Effect of Intake Pressure

Similar to increasing intake temperature, increasing intake pressure broadly decreased the critical compression ratio for all fuels, as shown in Fig. 11. Interestingly, increasing intake pressure to 2.0 bar resulted in lower critical compression ratios than increasing intake temperature to 200 °C, meaning that the fuel reactivity was more sensitive to changes to intake pressure than to intake temperature. Trends of critical compression ratio for E10, iButA15.5, and iButA16.3-Tol-nHep7 are similar for increasing intake pressure, as they are for increasing temperature; E10 and iButA15.5 remain together and in the middle of the pack, iButA16.3-Tol-nHep7 maintains highest critical compression ratio throughout. However, increasing intake pressure does not change the relative critical compression ratios of the remaining three fuels in relation to one another. While increasing intake temperature moved iPentA18.4-IOct15 from the most reactive to least reactive (compared to iButA15.5-DIIB-nHep5 and Prenol 16.7), iPentA18.4-IOct15 remains the most reactive fuel at all intake pressures (Figs. 10 and 11).

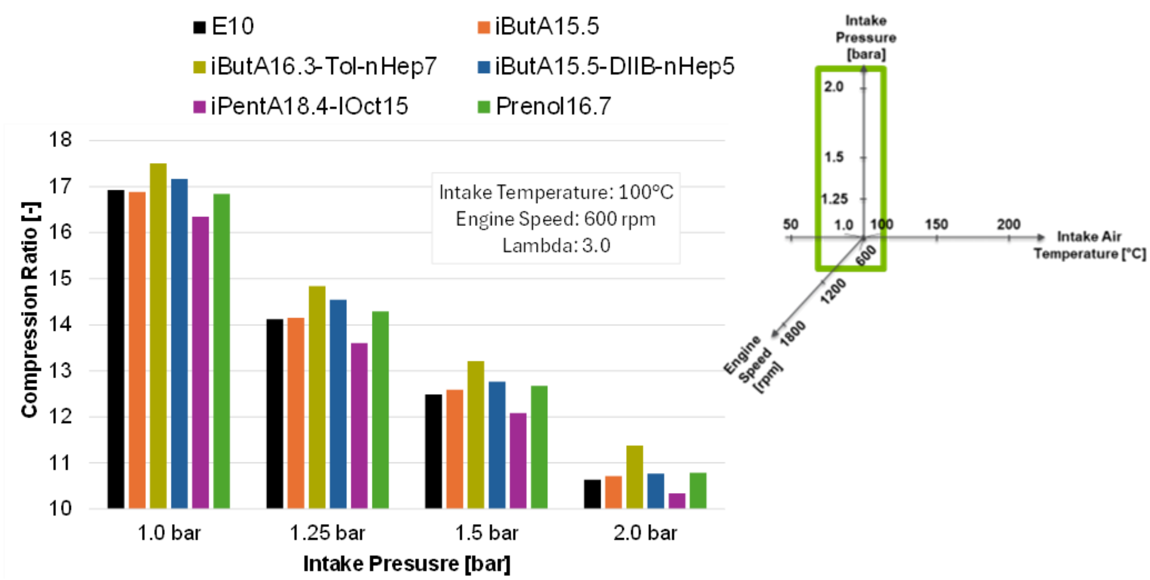


Figure 11: Effect of intake pressure on critical compression ratio

4.2.3 Effects of engine speed

Figure 12 shows that increasing engine speed increased critical compression ratio non-linearly. There was a significant increase in critical compression ratio when increasing engine speed from 600 RPM to 1200 RPM, but a much more modest increase in critical compression ratio from 1200 RPM to 1800 RPM. Considering individual fuels from left to right, E10 and iButA15.5 move from a median critical compression ratio at low engine speeds to the highest critical compression ratios at high engine speeds; additionally, critical compression ratio for iButA15.5 drops a bit below E10 as engine speed increases. The aromatic fuel blend (iButA16.3-Tol-nHep7) surrenders its position of highest critical compression ratio to E10 at the higher engine speeds. Finally, trends for the remaining three fuels are much like the temperature sweep; as engine speed increases iPent18.4-IOct15 goes from being most reactive at low speed, to the least reactive at high temperatures, trading relative position with iButA15.5-DIIB-nHep5 and Prenol 16.7.

Understanding the trends due to changing engine speed is a bit more challenging than a thermodynamic condition change, like temperature or pressure, because engine speed alters several parameters simultaneously. It may be most obvious that the residence time is decreased for each cycle, requiring more energy input (via increased compression ratio) to achieve the same combustion/knocking threshold. Additionally, trapped residual exhaust gases are expected to increase as there is not as much time for gas exchange through the intake/exhaust valves. More exhaust gases in the cylinder not only implies an increase in dilution (inert) species, but also heats the charge mixture more than at lower engine speed. The heating effect of the residual exhaust gases may be responsible for the similar trend with iPent18.4-IOct15 across increasing temperatures (Fig. 10) and engine speed (Fig. 12). Lastly, increasing engine speed is known to enhance turbulence and diffusivity of the charge mixture which influences flame propagation characteristics. The combination of these thermodynamic impacts are challenging to unravel (hence why engine experiments are necessary) but may in some way provide explanation for the non-linear behavior noted in the results of increasing speed.

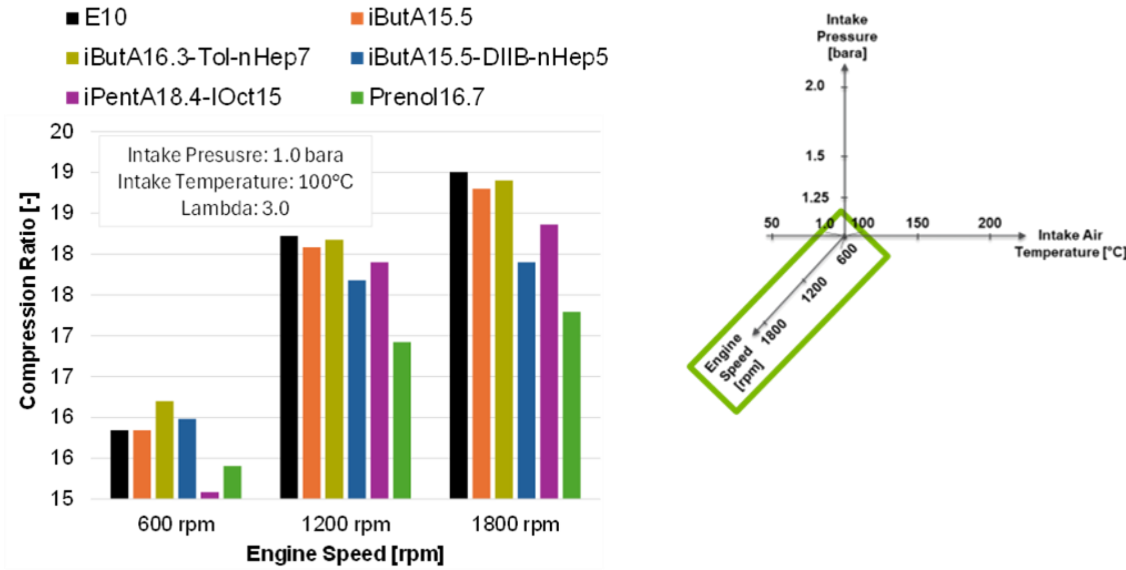


Figure 12: Effect of engine speed on critical compression ratio

4.2.4 Effect of excess air ratio (lambda)

To evaluate the effect of lambda, three engine operating points were selected from the test matrix for a sensitivity analysis when increasing lambda from 3 (baseline) to 4 (increased excess air). Figure 13 shows the sensitivity of Critical Compression Ratio to this change in lambda by plotting the *delta* of compression ratio. Consider the baseline case in Fig. 13 (100°C, 600 RPM, 1 bar), where the delta of compression ratio varied between 1.5 and 1.8 across the different test fuels, showing that the chemical composition of the fuels impacted their lambda sensitivity under the baseline conditions. In addition to the HCCI Critical Compression Ratio ratings at different engine operating conditions, as discussed in previous sections, the lambda sensitivity is a fuel property measured through HCCI ratings on a CFR engine that could suggest additional autoignition reactivity characteristics when the fuels are injected and combusted under stratified conditions. This information could be useful in designing fuels to enhance ACI engine performance by developing control strategies for commercial ACI engines to enhance low-load and cold-start reactivity or mitigate combustion noise under high-load and more reactive cylinder conditions.

As expected, all operating conditions and fuels are more resistant to autoignition (i.e., have higher critical compression ratios) when lambda is increased. In general, the highest lambda sensitivity occurs at baseline conditions. Interestingly, the fuels demonstrated sensitivity to lambda at baseline conditions and the high speed test condition, whereas the sensitivity to lambda between each fuel was quite similar at increased intake pressure (2 bar). The relative fuel insensitivity to lambda for the high intake pressure case suggests that boost pressure plays a more dominant role in reactivity than fuel chemistry at these engine operating conditions. The 1800 RPM case showed the lowest magnitude of lambda sensitivity in general, and yet the greatest variability in lambda sensitivity between fuels. The high degree of variability may be due to the combination of thermodynamic changes which occur at increased engine speed such as enhanced turbulence and increased exhaust residual fraction, as discussed in Sec. 4.2.3.

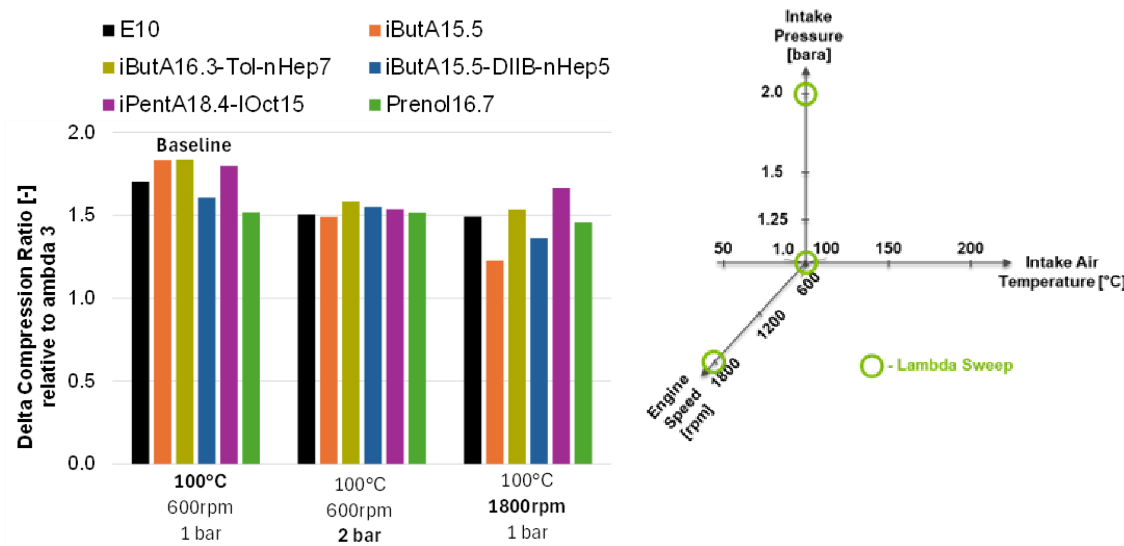


Figure 13: Effect of lambda on critical compression ratio, shown as the delta of critical compression ratio when changing lambda from 3 to 4, at select engine operating conditions.

4.3 Results, Phase 3

The focused set of fuels were also tested in low load GCI operation on a HD-SCE and similar trends were observed as in the CFR engine HCCI fuel ratings (Fig. 14). Replacing 10 vol% ethanol (baseline 87 AKI E10 gasoline) with 18.4 vol% isopentanol improved low load operability on the HD-SCE across its full test matrix and correlated with a higher reactivity (lower Critical Compression Ratio) on the CFR engine likewise across all of test conditions. When replacing ethanol with isobutanol, HD-SCE low load operation was improved across all low load GCI test conditions. However, under CFR HCCI test conditions, the isobutanol-blended gasoline showed only slightly higher (if not similar) reactivity as the baseline ethanol-blended gasoline across all HCCI rating conditions.

Interestingly, similar trends were observed of the prenol-blended gasoline relative to the E10 baseline gasoline on both engines. The HD-SCE engine testing showed improved GCI low load performance for the prenol blend over the E10 gasoline only under the high temperature test condition, whereas CFR HCCI ratings showed the most significant increase in prenol-blended gasoline reactivity over the baseline E10 gasoline when the CFR intake temperature was increased (and derivatively the engine speed increase).

When considering the variations of isobutanol-blended gasolines, where the base gasoline had elevated aromatic (toluene) or olefic (diisobutylene) content, some consistent findings between the HD-SCE and CFR HCCI ratings were observed as well. On the HD-SCE engine, addition of aromatic or olefin adversely affected the low load GCI operation relative to the isobutanol-gasoline blend without aromatic or olefin added. This trend correlated with the aromatic and olefinic isobutanol-gasoline blends showing reduced HCCI reactivity on the CFR engine for intake temperatures of 50-100 °C, and across all intake pressure test points (which were at 100 °C intake temperature). Across all test conditions on the HD-SCE, the aromatic isobutanol-gasoline blend had worse low load GCI performance than the E10 baseline gasoline, which correlated to that fuel also having lower CFR HCCI reactivity (higher Critical Compression Ratio) than the E10 baseline gasoline across all intake temperature and intake pressure sweep test conditions.

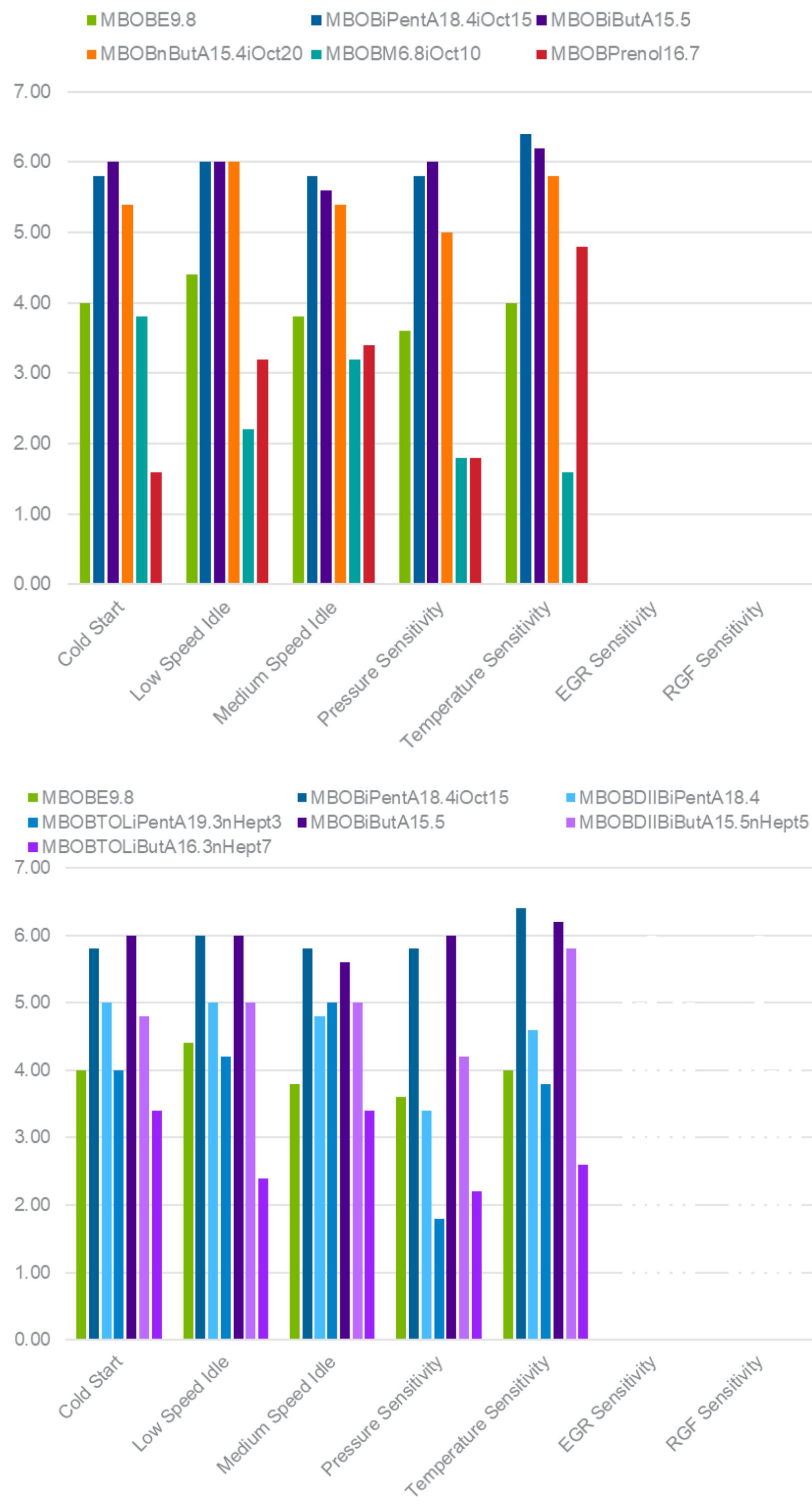


Figure 14: HD-SCE operability metric across fuel and conditions

5. Summary and Conclusions

The CFR engine was upgraded substantially to extend its testing capabilities to ACI relevant conditions, while maintaining backward compatibility for its intended purpose for evaluating knocking propensity and octane number of fuels in spark ignition engines. The unique experimental facility was utilized to study the impact of base fuel composition and blended alcohols on compression-ignition reactivity. First, an extensive set of fuels were tested at fixed engine operating conditions, revealing that the autoignition propensity of fuels differed from their RON, MON, or AKI knocking propensity metrics. A comprehensive experimental matrix was then devised to evaluate a focused set of fuels across a wide range of engine operating conditions relevant to ACI engine operation. In particular, a range of intake pressures, intake temperatures, engine speeds, and lambdas were tested with the selected fuels. Finally, the focused set of fuels were evaluated in an application-relevant HD-GCI engine platform. The HD-GCI engine tests revealed similar fuel ranking trends as the CFR engine testing, confirming that autoignition measurement trends of different fuel blends transcend the engine hardware. From this study, the following was concluded:

- At constant AKI and oxygen content, different alcohol fuel blends, including varied aromatic and olefinic compositions, can change autoignition reactivity, indicating a need for a compression ignition fuel rating for ACI engines.
- The response of autoignition reactivity to increasing intake temperature was varied for the different fuel blends. For example, the isopentanol-based gasoline (iPent18.4-IOct15) was the most reactive fuel at low temperature, and among the least reactive at high temperature, showing the importance of understanding temperature effects.
- Intake pressure increased the reactivity (reduced the Critical Compression Ratio) of all fuels similarly; not affecting the relative reactivity rankings between the fuels.
- Generally across all the fuels, a 1 bar increase to intake pressure showed a stronger increase in reactivity (evidenced by reduction to Critical Compression Ratio) than a 150 °C increase to intake temperature. This shows that from an ACI engine controls standpoint, intake pressure is a more sensitive control on 87 AKI gasoline autoignition reactivity than intake temperature.
- Increasing engine speed resulted in a non-linear increase in Critical Compression Ratio and a similar variation in reactivity ranking of the fuels as increased intake temperature. It is hypothesized that the charge temperature is increased at faster

engine speeds due to the corresponding increased retention of hot residual exhaust gases.

- Aromatic fuel blends were found to be consistently most resistant to autoignition.
- A strong correlation of CFR HCCI fuel reactivity rankings with GCI low load performance on a heavy-duty single-cylinder engine (HD-SCE) was observed, providing additional evidence of the value of CFR rating of gasoline-like fuels in advanced compression ignition combustion modes.

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7. Nomenclature

ACI	Advanced Compression Ignition
AKI	Anti-Knock Index
CFR	Cooperative Fuel Research
DIIB	Diisobutylene
E	Ethanol
GCI	Gasoline Compression Ignition
HCCI	Homogeneous Charge Compression Ignition
HD	Heavy-Duty
Hep	n-Heptane
iButA	Isobutanol
IMEP	Indicated Mean Effective Pressure

iPentA	Isopentanol
Iso	Isooctane
LD	Light Duty
MAPO	Maximum Amplitude of Pressure Oscillation
MBOB	Marathon Blendstock for Oxygenate Blending (gasoline)
MD	Medium-Duty
MM	Multi-Mode
MON	Motor Octane Number
nButA	n-Butanol
PPCI	Partially Premixed Compression Ignition
RCCI	Reactivity Controlled Compression Ignition
RON	Research Octane Number
RPM	Revolutions per Minute
SCE	Single Cylinder Engine
SCOTE	Single Cylinder Oil Testing Engine