

Significance of RON, MON, and LTHR for Knock Limits of Compositionally Dissimilar Gasoline Fuels in a DISI Engine

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ABSTRACT

Spark-ignition (SI) engine efficiency is typically limited by fuel auto-ignition resistance, which is described in practice by the Research Octane Number (RON) and the Motor Octane Number (MON). The goal of this work is to assess whether fuel properties (i.e. RON, MON, and heat of vaporization) are sufficient to describe the antiknock behavior of varying gasoline formulations in modern engines. To this end, the auto-ignition resistance of three compositionally dissimilar gasoline-like fuels with identical RON values and varying or non-varying MON values were evaluated in a modern, prototype, 12:1 compression ratio, high-swirl (by nature of intake valve deactivation), directly injected spark ignition (DISI) engine at 1400 RPM. The three gasolines are an alkylate blend (RON=98, MON=97), a blend with high aromatic content (RON=98, MON=88), and a blend of 30% ethanol by volume with a gasoline BOB (RON=98, MON=87; see [Table 2](#) for details).

The preliminary findings of this work are that RON and MON, when coupled with latent heat of vaporization information, are sufficient to describe the auto-ignition resistance of a fuel to a degree such that knock-limited combustion phasing shows no measurable differences. While the tested fuels yielded no inconsistencies between their ratings (RON and MON) and properties (latent heat of vaporization) and their performance in a DISI engine, measurable differences were found among the three tested fuels. Specifically, the manner in which the fuels obtained knock-resistance varied, be it through thermal tolerance, charge cooling, or lack of charge-heating Low-Temperature Heat Release (LTHR). In addition, the fuels' knock-limited combustion phasing responses to variations in intake pressure and intake temperature varied with their thermal tolerance and tendency towards LTHR. Yet these dissimilar behaviors combine to produce similar anti-knock qualities and engine performance for naturally-aspirated operation.

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INTRODUCTION

Gasoline Spark-Ignition (SI) engines are the dominant form of combustion engine in the U.S. light-duty market, and have been for many decades. A significant impediment to SI engine efficiency is auto-ignition of the end-gas prior to consumption of the end-gas by deflagration-based combustion [1]. Auto-ignition of the end-gas typically produces a sharp, metallic noise referred to as knocking, and can cause problems with vehicle Noise, Vibration, and Harshness (NVH), as well as problems with premature engine failure.

Knocking is fundamentally caused by compression of the end-gas, which raises the temperature and pressure of the end-gas to the point of auto-ignition. The compression heating is due to the pressure rise caused by piston motion in combination with an expansion of the burned gases as the flame propagates. Knocking is avoided in a number of ways, which typically fall into two categories: alterations to the engine or engine operating conditions which reduce peak temperatures and pressures faced by the end-gas, or selection of a fuel that is more resistant to auto-ignition. This study focuses on

understanding the resistance of different fuels to auto-ignition, in order to enable the use of more efficient operating conditions in modern SI engines.

Knocking hampers SI engine efficiency by limiting the compression ratio employed in production engines; analysis of the ideal Otto thermodynamic cycle shows the compression ratio has an important role in determining the efficiency of Otto engines, as seen in [Eq. 1](#).

$$\eta = 1 - (1/(CR^{(\gamma-1)}))$$

Eq. 1

By employing fuels which are more resistant to end-gas auto-ignition, SI engines can be produced and calibrated to be more efficient by making use of higher compression ratios and optimal spark timing.

This study is part of a broader research program named Co-Optimization of Fuels and Engines (Co-Optima) [2], run by the Department of Energy, whose goal is to identify opportunities that arise when fuels and engines are co-optimized. This study investigates the important hypothesis used in the Co-Optima project,

namely that fuel properties are sufficient to predict the behavior of fuels in engines. An example of this hypothesis is that a fuel's RON [3], MON [4], and latent Heat of Vaporization (HoV) describe the fuel's resistance to auto-ignition in a SI engine relative to other fuels. To test this hypothesis, this study uses three carefully selected fuels, which share the same RON, but vary MON and HoV.

A significant body of work exists which relate RON and MON ratings of fuels to SI engine performance [5, 6, 7]. In particular, the Octane Index [8, 9, 10] has been shown to reasonably predict the knock resistance of fuel in engines; this method estimates knock resistance based on weighting RON and MON ratings via information specific to the engine and operating point of interest. While this method works well to an engineering approximation, it is not clear that this method works well with non-petroleum based fuels, or fuels with varying HoV's [11]. Thus, for the purpose of evaluating novel, bio-derived fuel molecules as part of the Co-Optima project [2], a deeper understanding of the role of fuel properties and specifications on knock-resistance is desired.

This study assesses the knock-resistance and underlying phenomena of three gasoline-type fuels, which will be described in detail in the following section. It will be shown that these fuels are resistant to end-gas auto-ignition for different combinations of chemical auto-ignition resistance and charge cooling effects, yet behave similarly in the engine as would be expected by their matching RON and similar MON ratings.

EXPERIMENTAL SETUP

Research Engine Facility

The engine used for the experiments is a single-cylinder four-valve research engine that can be set up in two configurations: an all-metal configuration for continuously fired performance testing, or in a nearly identical optical configuration for imaging studies. All tests here were conducted with the all-metal configuration, using a water-cooled metal cylinder and oil-lubricated metal piston rings, and run at an engine speed of 1400 RPM. The piston has a moderately deep piston bowl to aid the stratification of fuel for spray-guided stratified-charge operation, *e.g.* Ref. [12]. However, for these tests the fuel was injected during the intake stroke to generate a well-mixed charge. Figure 1 shows a cross section of the combustion chamber with the piston at TDC. The long-reach spark plug allows the spark plasma to develop in a central location of the combustion chamber, which should be particularly beneficial for lean operation; however, in this work only stoichiometric un-diluted conditions were tested. This long-reach spark plug is used with a high-energy inductive ignition system, as described in the "Conventional Inductive Spark System" section of this manuscript.

Engine data are given in Table 1. The engine was fueled using a Bosch 8-hole step-hole Valve Covered Orifice injector. The injector was oriented such that two of the fuel sprays straddled the spark-plug gap of the commercial long-reach spark plug. For all data, the

phasings of the cam shafts relative to the crank shaft were maintained constant. The cam shafts were phased to provide both low residual levels and high volumetric efficiency. A graphical representation of the valve lifts can be found in Ref. [13]. It should be noted that one intake valve was deactivated to increase in-cylinder swirl and tumble levels (see Table 1). In this study, the crank angles (CA) are referenced as after top dead center of the combustion stroke, aTDC. Exhaust-gas residual levels of this engine vary as a function of intake and exhaust pressure; in this study the residual gas level ranged from a maximum of 7% at a throttled, 60 kPa intake pressure condition, to a minimum of 3% at a lightly boosted 110 kPa intake pressure. The air was metered into the intake system using a sonic-flow nozzle.

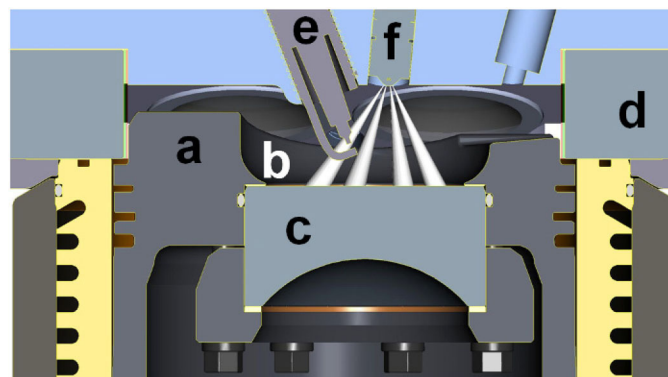


Figure 1. Cross-section of combustion chamber at TDC: a - piston, b - piston bowl, c - piston-bowl window, d - pent-roof window, e - spark plug, and f - fuel injector. Metal window blanks were used in this study.

Table 1. Engine Specifications

Displacement.....	0.552 liters
Bore	86.0 mm
Stroke	95.1 mm
Connecting Rod Length	166.7 mm
Geometric Compression Ratio.....	12:1
Intake Valve Diameter	35.1 mm
Intake Valve Angle Relative Cylinder Axis	18°
Exhaust Valve Diameter	30.1 mm
Exhaust Valve Angle Relative Cylinder Axis.....	16°
Swirl / Tumble Index (one intake valve deactivated).....	2.7 / 0.62
Fuel Injector.....	Bosch 8-hole solenoid-type
Hole Orientation.....	Symmetric with 60° included angle
Hole Size	Stepped-hole, min. dia. = 0.125 mm

The exhaust gas flow was diluted with extra air using nozzles at the entry point of the exhaust tank. This was done to limit the exhaust gas temperature in the tank and to lower the dew point of the exhaust gases to avoid loss of unburned hydrocarbons (HC) and water due to condensation in the unheated sample lines. With precisely known exhaust dilution, the measured exhaust composition was back-corrected to engine-out mole fractions. A Horiba MEXA-584L emission analyzer measured CO, CO₂ and HC. O₂ was measured with a CAI 600PP gas analyzer. NO_x was measured with a CAI 600CLD gas analyzer. Exhaust smoke was measured with an AVL 415S smoke meter.

Conventional Inductive Spark System

The conventional inductive system was supplied by Bosch. The spark coil (model ZS-L 1x1E) can provide relatively high spark energy. For all the tests reported here, the charging time of the primary coil was set to 5 ms. According to measurements by Bosch, this results in a spark energy of nominally 106 mJ being delivered from the secondary high-voltage coil. The secondary coil was connected to an NGK spark plug featuring a long-reach single-point J-gap. The spark gap width was adjusted to 1.0 mm prior to the engine tests.

Experimental Procedure and Data Analysis

For each operating point with the all-metal engine configuration, the engine is allowed to run for several minutes until all measured parameters are stable, at which point data are acquired. Fuel-flow rate and thermocouple readouts are averaged over one minute. The in-cylinder pressure, spark current, intake and exhaust pressure, and fuel pressure are acquired for 500 consecutive cycles using 0.1°C resolution. For the in-cylinder pressure, an uncooled Kistler 6125C piezoelectric sensor is used in combination with a Kistler 5010B charge amplifier. Day-to-day repeatability is very good, with variations of average indicated mean effective pressure (IMEP) of less than 2%.

The apparent heat-release rate (AHRR) is computed from the in-cylinder pressure for each individual cycle using a constant ratio of specific heats ($\gamma = 1.33$) following [1]. The value of γ was chosen to yield a net-zero AHRR near the end of the compression-stroke prior to combustion. For computing combustion-phasing metrics like the 50% burn point (CA50), the AHRR is integrated over the crank-angle range for which AHRR is positive. For all data presented, this computation of burn points is performed in a conventional way, whereby the integral of AHRR is scaled so that it rises from 0 to 100% for every cycle, irrespective of the actual η_{comb} .

Fuels

This study focuses on the influence of fuels composition on knock-limited operation of a directly-injected spark-ignition (DISI) engine. The three fuels used in this study were carefully designed for this purpose. The fuels were procured from Gage Products Company, who blended the fuels from refinery streams to provided specifications. Upon receipt, the fuels were sent to Southwest Research Institute (SwRI) for analysis [14], which included RON and MON testing per ASTM specifications, as well as a detailed hydrocarbon analysis (DHA), and heat of combustion measurements. Selected values from these analyses are presented in Table 2.

The three fuels used in this study have been given names for the convenience of the reader; these names are based on the composition of the fuels. For instance, the fuel named “Alkylate” is primarily composed of branched, saturated hydrocarbons (alkanes). Similarly, the “E30” fuel is comprised of 30% ethanol on a volume basis, and the “High Aromatic” fuel is comprised of a large fraction (31% by volume) of aromatic hydrocarbons.

The three tested fuels were specified to have RON ratings of 98 ± 0.5 ; analysis by SwRI found all three fuels met this specification within the tolerance of the RON test (0.3 ON). The RON rating was chosen as a baseline for the fuels due to its relevance to modern SI engines, while the MON ratings of the fuels were intentionally varied to provide two Octane Index [8] values for any condition not described by $K = 0$. The Octane Index is shown in Eq. 1, and supported by Eq. 2. From these two equations, it may be seen that $OI (K=1) = MON$ while $OI (K=0) = RON$. The variation in the OI values of the fuels were achieved by specifying identical Octane Sensitivities for the two high-sensitivity fuels (High Aromatic and E30).

$$OI = (1 - K) \cdot RON + K \cdot MON = RON - K \cdot S \quad (1)$$

$$S = RON - MON \quad (2)$$

Table 2. Selected fuel properties and ratings for the three fuels used in this study.

	<i>Alkylate</i>	<i>E30</i>	<i>High Aromatic</i>
RON	98	98	98
MON	97	88	87
AKI (R+M)/2	97	93	93
Sensitivity (RON - MON)	1	10	11
T10 (°C)	93	61	59
T50 (°C)	100	74	108
T90 (°C)	106	155	158
TF (°C)	161	204	204
Aromatics (Vol. %)	0	8	31
Olefins (Vol. %)	0	5	4
Parafins (Vol. %)	100	57	65
Ethanol (Vol. %)	0	30	0
Net Heat of Combustion (MJ/kg)	44.5	38.2	43.0
Assumed Latent Heat of Vaporization (kJ/kg)	350.0	533.6	350.0
Average Molecular Formula	C: 7.76 H: 17.45	C: 4.49 H: 9.87 O: 0.5	C: 6.92 H: 12.41

From Table 2, the E30 and High Aromatic fuels can be seen to have similar distillation curves, with nearly identical T10, T90, and TF temperatures that are within the gasoline boiling range. However, the Alkylate fuel does not exhibit a wide boiling range, as it is primarily composed of iso-octane; this is dissimilar from document gasoline.

and reminiscent of Primary Reference Fuels, but this distillation behavior is assumed to be of minor importance for this study, due to the well-mixed early-injection strategy employed.

The fuels are assumed to have varying HoV values; this has not been measured due to the difficulty in measuring HoV for multi-component mixtures. For this study, the HoV of the Alkylate and High Aromatic fuels are assumed to be similar to commercial petroleum-based gasoline (350 kJ/kg), while the E30 is assumed to have a HoV value based on linear blending of ethanol with gasoline (533.6 J/kg). This assumption is used by GT Power to calculate the charge-cooling due to the fuel's evaporation in the combustion chamber during the intake stroke.

Operating Conditions

Knock-limited CA50's (KL-CA50) were measured for each fuel over a range of operating conditions which were chosen for their relevance to modern and future engine design. These conditions are presented in Table 3. The knock-resistance of each fuel (as evaluated by KL-CA50) was tested with intake pressures ranging from 60 kPa to 110 kPa at 30 °C intake temperature, and 60 kPa to 100 kPa at 60 °C and 90 °C intake temperature (intake temperatures were measured in the intake runner). These intake conditions yielded a range of KL-CA50's from overly advanced at 60 kPa (combustion phasing advanced from MBT timing: 8 – 10 CAD aTDC) to highly retarded at 110 kPa (combustion phasing approaching 30 CAD aTDC). These conditions could be encountered by a future high-efficiency, high compression ratio, naturally-aspirated DISI engine when using a highly knock-resistant fuel similar to those used in this study. Also of interest are conditions that may be encountered by future high-efficiency boosted DISI engines; however, this is beyond the scope of the present study, though plans are in place to investigate these conditions (see Future Work section at the end of this manuscript).

Table 3. Operating conditions for fuel, intake pressure, and intake temperature sweeps of KL-CA50.

Variable	Range
Fuel	Alkylate, High Aromatic, E30
Intake Temperature	30, 60, 90 °C
Intake Pressure	60, 80, 100, 110 (30 °C only) kPa

Knock Intensity Calculation

To quantify the acoustic noise generated by rapid autoignition-based combustion of the end-gas, an in-house developed metric named Knock Intensity (KI) was used. It is based on the measured in-cylinder pressure, which is processed on a cycle-by-cycle basis over several steps.

The measured pressure trace was first low-pass filtered (<1.5 kHz). This low-pass filtered pressure trace was then subtracted from the unfiltered trace, effectively rendering a high-pass filtered pressure trace. Lastly, using Fourier decomposition, the energy content in the 0 – 80 CAD aTDC range was summed over the frequency range of 5 – 28 kHz. The crank-angle range was limited to increase signal-to-noise of this KI metric. The specific frequency range was chosen to

capture the pressure oscillations related to knocking combustion, but to avoid those oscillations related to noise in the sensor or data acquisition system (> 28 kHz) or to the piston motion and deflagration-based combustion (< 5 kHz). The reported KI values correspond to the average over 500 cycles. Figure 2 provides examples of the frequency content of lightly-knocking pressure traces for the three tested fuels. Also included are their respective computed KI's and Combustion Noise Levels (CNL's) [15]. This figure illustrates the chief oscillatory frequencies due to knock and normal combustion. It may be seen that these three fuels exhibit similar frequency content, allowing the use of a fixed frequency range for this analysis.

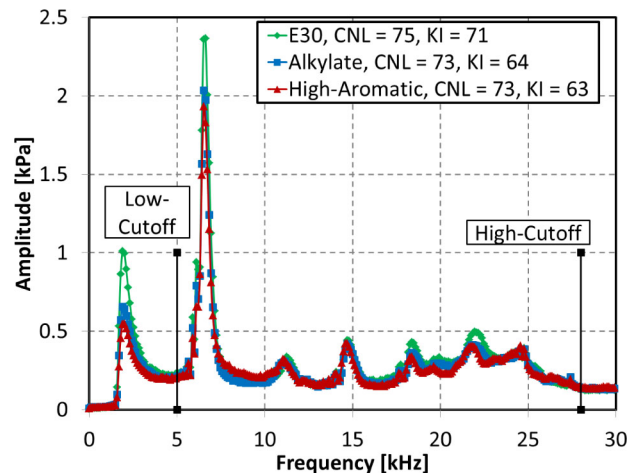


Figure 2. Frequency content of three measured pressure traces under "light" knocking conditions, yielding KI values that correspond to Knock-Limited combustion phasing. Also shown are the low- and high-frequency cutoffs in relation to the frequency range which contributes to the KI value (5 – 28 kHz).

Knock-Limited CA50 Measurement Procedure

A key metric of this study are the Knock-Limited Combustion Phasings (KL-CA50's) of each fuel over a range of operating conditions. Each KL-CA50 was measured by fixing intake pressure and temperature, and varying spark timing until the steady-state average combustion phasing resulted in a KI between 60 and 80, with a value of 70 being the target. At this KI level, the engine operation exhibited knock that was audible above the mechanical noise of the engine for a large fraction of the cycles. In addition, a large fraction of the cycles display a second AHRR peak, corresponding to the enhanced combustion rate due to end-gas autoignition. As such, the engine operation was harsher than what is tolerable for automotive engine calibration, but such operation with clearly distinguished knock facilitated this parametric knock study.

Figure 3 shows that the KI values obtained were highly dependent on CA50 under the investigated conditions. To this end, spark timing was controlled in 0.1 CAD increments, which enabled CA50 control on a similar scale. Figure 3 also shows that KI varied significantly over a range of 1 CAD, indicating that small variations in KI among the measured operating points did not significantly affect the determination of KL-CA50. Even so, it should be noted that knock statistics vary both with fuel type and operating conditions, as discussed the last result section.