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# Understanding chemistry-specific fuel differences at a constant RON in a boosted SI engine

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ABSTRACT

The goal of the US Department of Energy Co-Optimization of Fuels and Engines (Co-Optima) initiative is to accelerate the development of advanced fuels and engines for higher efficiency and lower emissions. A guiding principle of this initiative is the central fuel properties hypothesis (CFPH), which states that fuel properties provide an indication of a fuel's performance, regardless of its chemical composition. This is an important consideration for Co-Optima because many of the fuels under consideration are from bio-derived sources with chemical compositions that are unconventional relative to petroleum-derived gasoline or ethanol. In this study, we investigated a total of seven fuels in a spark ignition engine under boosted operating conditions to determine whether knock propensity is predicted by fuel antiknock metrics: antiknock index (AKI), research octane number (RON), and octane index (OI). Six of these fuels have a constant RON value but otherwise represent a wide range of fuel properties and chemistry. Consistent with previous studies, we found that OI was a much better predictor of knock propensity that either AKI or RON. However, we also found that there were significant fuel-specific deviations from the OI predictions. Combustion analysis provided insight that fuel kinetic complexities, including the presence of pre-spark heat release, likely limits the ability of standardized tests and metrics to accurately predict knocking tendency at all operating conditions. While limitations of OI were revealed in this study, we found that fuels with unconventional chemistry, in particular esters and ethers, behaved in accordance with CFPH as well as petroleum-derived fuels.

## 1. Introduction

The US Department of Energy Co-Optimization of Fuels and Engines ("Co-Optima") initiative aims to foster the codevelopment of advanced fuels and engines for higher efficiency and lower emissions. A guiding principle of Co-Optima is the central fuel properties hypothesis (CFPH), which states that fuel properties provide an indication of the performance and emissions of the fuel, regardless of the fuel's chemical composition. CFPH is important because many of the fuel candidates being investigated in the Co-Optima initiative are bio-derived compounds with oxygen-containing functional groups not typically associated with commercial transportation fuels. The purpose of this investigation was to determine whether the fuel properties associated with knock resistance, namely the research octane number (RON) and the motor octane number (MON), are consistent with CFPH.

More than a century ago the complex abnormal combustion phenomenon in spark ignition (SI) engines known as "knock" was attributed to end-gas autoignition [1]. However, barriers still exist to developing a fully detailed understanding of knock, which is problematic because it continues in higher efficiency SI engines. Recent downsizing and downspeeding trends with cars and trucks [2] exacerbate the issue by driving engines toward higher power density and higher load duty cycles, where knock is more problematic.

In the United States, gasoline is sold with an antiknock index (AKI) rating that is the average of the RON and the MON. The RON test was originally introduced in 1928, but the MON test was not developed until 1932, motivated by a finding that real-world fuels were underperforming the certification results by 2.5–3.0 octane rating points [3]. The MON test introduced a higher engine speed (900 rpm vs. 600 rpm) and a higher intake temperature (149 °C downstream of the carburetor

*Abbreviations:* AKI, antiknock index; $aTDC_f$, after top dead center firing; CA, crank angle; CA05, crank angle of 5% heat release; CA50, crank angle of 50% heat release; CFP, central fuel properties hypothesis; DI, direct injection; EA, ethyl acetate; EGR, exhaust gas recirculation; HoV, heat of vaporization; IMEP, indicated mean effective pressure; KI, knock intensity; KLSA, knock-limited spark advance; LHV, lower heating value; LTHR, low temperature heat release; MB, methyl butyrate; MON, motor octane number; NTC, negative temperature coefficient; OI, octane index; PRF, primary reference fuel; RON, research octane number; RVP, Reid vapor pressure; S, octane sensitivity; SI, spark ignition; TDC, top dead center

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vs. 52 °C upstream of the carburetor). The MON test conditions were an effort to address the reality that the relative ranking of knock resistance among a set of fuels changes as the engine conditions change. As a measure of this, the concept of octane sensitivity (S), defined as the difference between RON and MON, was introduced.

Leppard [4] investigated the chemical origin of S, focusing on different chemical classes. For alkanes, there is a two-stage ignition process: low-temperature heat release (LTHR) followed by a negative temperature coefficient (NTC) region wherein the reaction rate becomes inversely proportional to the temperature. Following these processes is a high-temperature heat release event. The chemical origins and dependencies of the two-stage ignition process were later elucidated in the development of chemical kinetic mechanisms for the primary reference fuels (PRFs) n-heptane [5] and iso-octane [6], the paraffinic fuels that define the RON and MON scales. The PRF fuels exhibit similar knocking behavior in the RON and MON tests even though the intake manifold temperature increases significantly, thus the NTC behavior makes the fuels insensitive to changes in intake temperature. Because other paraffinic fuels also exhibit two-stage ignition behavior, low S is ubiquitous among paraffinic fuels. In contrast, Leppard [4] showed that neither aromatics nor olefins exhibited the two-stage ignition behavior, and as a consequence, these fuels have high S. Recently, the chemical origins of the fuel S findings of Leppard have been studied by Westbrook et al. [7], illustrating that fuel S effects can be explained through local electron delocalization.

Independent kinetic modeling studies performed by Yates et al. [8] and Mehl et al. [9] demonstrated that the RON and MON tests represented two different pressure-temperature trajectories. The MON trajectory had a higher temperature at a given pressure and consequently avoided the pressure-temperature conditions that resulted in LTHR before encountering the pressure-temperature conditions of the NTC region. In contrast, the RON trajectory had a lower temperature at a given pressure, leading to conditions that yield a much stronger LTHR event prior to entering the pressure-temperature conditions of the NTC region. Thus, the relative knock-resistance order of fuels can change depending on the pressure-temperature trajectory, and this ranking is largely dependent on S. Further, Yates et al. [8] showed that carbureted engines operate at pressure-temperature trajectories between RON and MON, port fuel injection engines operate closer to the RON trajectory, and boosted direct injection (DI) engines can operate at pressure-temperature trajectories outside the bounds of RON and MON. While Yates et al. [8] describe these engine technologies in terms of their fueling technologies, the movement toward the RON trajectory can be attributed to a variety of technologies that reduce the temperature of the charge at intake valve closing, with engine breathing technologies being particularly important.

To relate the specific performance of an engine and fuel to the RON and MON tests, Kalghatgi [10] pioneered a practical method to correlate the RON and MON values to knock-limited spark advance (KLSA). This method requires a parameter, K, which is dependent on the engine operating conditions, to act as a weighting factor between RON and MON. The resultant octane index (OI), (1), correlates to the actual knock propensity of the fuel much more strongly than either RON or MON [11,12]. This allows the relative knock resistance of fuels to be determined at conditions in real engines which differ from the RON and MON tests, but a statistical fit from experimental data is required to determine K. The OI correlates to knock in boosted SI engines [13,14], which typically have a pressure-temperature trajectory that is “beyond RON,” which for a given cylinder pressure, corresponds to a lower temperature than the RON test, and in homogeneous charge compression ignition engines [15–18], which have a pressure-temperature trajectory that is “beyond MON,” which for a given cylinder pressure, corresponds to a higher temperature than the MON test.

$$OI = RON - K * S \quad (1)$$

In this study we sought to determine whether OI adequately explained the knock behavior using a set of seven fuels under boosted conditions in an SI engine equipped with DI fueling. Three of the fuels investigated are bio-blendstock candidates that are potentially of interest to Co-Optima and represent unconventional fuel chemistries for SI engines. To assess fuel performance over a broad set of intake conditions, the engine was operated over a range of backpressure, exhaust gas recirculation (EGR), and intake manifold temperatures at the same nominal fueling rate.

**Table 1**
Engine geometry.

| Parameter | Value |
|---|---|
| Bore × Stroke (mm) | 86.0 × 86.0 |
| Conrod length (mm) | 145.5 |
| Wrist pin offset toward expansion stroke (mm) | 0.8 |
| Compression ratio (–) | 9.2:1 |
| Fuel injection system | Direct injection, side-mounted, production injector with opposite linear wall directed six-hole spray pattern |

## 2. Methods

### 2.1. Experimental facility

The experimental apparatus and much of the methodology used in this study have been previously reported [19]. A 2.0 L GM Ecotec LNF engine equipped with the production side-mounted DI fueling system was used for this investigation. Engine geometry details are presented in Table 1. The engine was converted to a single-cylinder engine by disabling cylinders 1, 2, and 3. The combustion chamber geometry and camshaft profiles were unchanged from the stock configuration.

The engine was operated using a laboratory fueling system with a pneumatically actuated positive displacement pump in conjunction with an electronic pressure regulator to provide fuel rail pressure. A constant fuel rail pressure of 100 bar was used throughout this study.

A laboratory air handling system was constructed to allow for external EGR while using a pressurized facility and achieving a flipped pumping loop where the exhaust pressure is lower than the intake pressure. To accomplish this, pressurized and dried facility air having < 5% relative humidity was metered to a venturi air pump using a mass air flow controller. The venturi created up to an 8 kPa pressure differential, with the vacuum side pulling EGR through an EGR cooler into the intake. A schematic of the air pump arrangement with the electromechanical backpressure and EGR valves is shown in Fig. 1. The desired intake manifold temperature was achieved regardless of the EGR concentration using the combination of an EGR cooler and an electrical heater upstream of the intake surge tank. The EGR used in this study was not treated with an exhaust catalyst before being recirculated to the intake. EGR was measured using a nonintrusive method that utilizes pressure-compensated wideband oxygen sensors in both the intake and exhaust.

A Drivven engine controller with the Combustion Analysis Toolkit package was used to control the engine and acquire crank angle – (CA)–resolved data; however, detailed analysis on reported data were performed using an in-house–developed code. For each condition tested, cylinder pressure, spark discharge, and camshaft position data were recorded at 0.2° CA resolution for 1000 sequentially fired cycles. Cylinder pressure was measured using a flush-mounted piezoelectric pressure transducer from Kistler (6125C), and camshaft position was recorded from the production hall-effect sensors. Fuel injection timing was started during the intake stroke and was held constant at 280° CA before firing top dead center (TDC). Spark timing was adjusted as needed to achieve the desired combustion phasing, and spark dwell was held constant with the stock ignition coil at 1.8 ms to maintain constant