Mapping K factor variations and its causes in a modern, spark-ignition engine

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Abstract

The Research Octane Number (RON) and the Motor Octane Number (MON) are used to characterize gasoline's knock resistance in spark ignition engines. The utility of these two metrics has been questioned with advancements in engine technologies that significantly change the thermochemical environment inside the cylinder. The Octane Index, $OI = (1-K) \cdot RON + K \cdot MON$, has therefore been proposed to characterize the knock resistance of modern engines where K weights the relative contribution of the RON and MON and is primarily determined by engine design and operating conditions. Quantifying this K factor is central to understanding a fuel's anti-knock performance in a modern spark-ignition (SI) engine.

This work therefore determines the map of K over engine operating conditions for a 2-litre, 4-cylinder turbocharged, gasoline direct-injection engine. To achieve this, a novel blending system for primary reference fuels (PRFs) was developed to determine K by matching the knock resistance of the 91.6-RON certification gasoline with a PRF at each operating condition. The K values are determined over the engine map with normal and high intake air and coolant temperatures. At normal operating temperature, K is negative at most knock-limited conditions, consistent with previous findings, whereas at high operating temperatures, K is mostly positive and, indeed, exceeds 1 near 8 bar BMEP and 3000 RPM, demonstrating the relevance of the MON at some conditions of practical significance. Further analysis is conducted using engine simulations to examine the relationship between K and end gas conditions, and a strong correlation is observed between K and the unburned gas temperature at the later stages of combustion. This correlation is argued to have a sound physical basis in the engine's thermochemistry, supporting the utility of this K factor method.

Keywords

Engine knock, octane number, octane index, K factor

1 Introduction

Fuel economy regulations have been consistently driving the development of more efficient spark-ignition (SI) engines [1-3]. The application of modern technologies, such as high compression ratio, turbocharging, engine downsizing and downspeeding, promotes the tendency of engine knock. Various measures have been implemented to control knock, principally spark timing retard and fuel enrichment at some conditions. However, these measures have negative effects on engine efficiency and exhaust emissions.

The knock resistance of a fuel is characterized by two octane numbers – the Research Octane Number (RON) [4] and the Motor Octane Number (MON) [5]. These are determined with the Cooperative Fuel Research (CFR) engine using standard methods (Table 1). The RON and MON are determined by referencing the knock resistance of a test fuel to that of Primary Reference Fuels (PRFs) at corresponding conditions. PRFs are binary mixtures of iso-octane and n-heptane with the former defining an octane number of 100 and the latter defining an octane number of 0. The octane number of a PRF mixture is defined as the volumetric fraction of iso-octane in the mixture. As shown in Table 1, the RON is tested at an overall lower intake temperature than MON, and fuel vaporization cooling further reduces the mixture temperature past the carburetor. For most practical fuels, the RON is higher than the MON, but for PRFs their RON and MON are defined to be the same. The difference between RON and MON is known as octane sensitivity ($S = RON - MON$). The origin of S lies in the different autoignition chemistry between PRFs and octane sensitive fuels [6-8] as well as the different physical properties such as heat of vaporization (HoV) [9, 10].

Table 1 The RON and MON rating conditions as specified by the ASTM [11, 12].

Condition	RON	MON
Engine Speed (RPM)	600	900
Intake Temperature (°C)	52 (Intake air)	149 (Intake air-fuel mixture)
Spark Timing (CAD bTDC)	13	14-26
Compression Ratio	Variable, 4-18	
Fuel supply	Carburetor	
Lambda	Adjusted to maximum knock intensity	
Intake pressure	Unthrottled	

Historically, the two octane tests were designed to bracket the operating conditions of typical engines in the 1930s, where higher RON and MON generally meant better anti-knock quality. However, modern engines with direct injection (DI), turbocharging and variable valve timing (VVT) have vastly different cylinder conditions from those in the octane rating tests. As a result, the relevance of RON and MON to modern engines has received significant attention. Various studies in gasoline turbocharged direct-injection (GTDI) engines found that fuels of higher RON and lower MON (i.e. higher S) showed higher knock resistance and therefore allowed engines to operate with higher efficiency at high-load conditions [13-18]. Vehicle tests reported similar trends, where the acceleration performance improved with fuels of high RON and low MON [15, 19, 20]. These findings indicate the relevance of RON and MON to knock resistance in modern SI engines should be re-evaluated.

An alternative metric, Octane Index (OI), was proposed by Kalghatgi in 2001 [20, 21] to characterize a fuel's actual anti-knock quality in modern engines. As given by Eq. 1, OI is a linear combination of the RON and MON. K is a weighting factor that is primarily dependent on engine design and engine operating conditions. For example, the anti-knock index (AKI) used in North America approximates the OI by evenly weighting the RON and MON to a fuel's actual anti-knock quality ($K = 0.5$). The OI concept therefore generally reflects a fuel's knock resistance relative to its RON and MON ratings. A more commonly used expression for OI is given by Eq. 2, where S is the octane sensitivity. For an octane sensitive fuel ($S > 0$), its OI can be larger than the RON (when $K < 0$), or smaller than the MON (when $K > 1$), or in between, depending on the engine operation conditions. For PRFs, the OI always equals the RON and MON because $S = 0$. Although K is irrelevant in this case, PRFs provide a valuable reference for K determination, as shown later.

$$OI = (1 - K) \cdot RON + K \cdot MON \quad \text{Eq. 1}$$

$$OI = RON - K \cdot S \quad \text{Eq. 2}$$

In principle, K can be used to quantify the relative significance of the RON and MON to SI engine combustion. For example, when K is greater than 0.5, the MON is more important than the RON, and the higher the MON, the stronger the knock resistance is (at that operating condition in that engine); however, when K is negative, a higher MON causes a lower OI. Indeed, previous studies in modern SI engines showed that K was negative at most high-load conditions and therefore concluded that fuels of lower MON were advantageous [15-17, 21-23]. However, in practical driving, engines primarily operate at part loads, and recent studies found that K could be positive at part-load, knock-limited conditions [24, 25]. Therefore, further study is needed to determine K over a wide range of conditions in modern SI engines.

The objective of this work, therefore, is to determine K values in the Octane Index model over the full operation map of a modern GTDI engine, including severe operating conditions that involve high intake air and/or high coolant temperatures. A novel fuel blending system is developed to continuously prepare and

supply PRF mixtures of the needed composition in real time to match the anti-knock performance of a 92 RON/83 MON gasoline, from which the K of each condition is determined. The obtained K dataset is used to generate a contour map of K overlaid on the engine operation map. The comprehensive dataset also enables statistical analysis for potential correlations between K and the end gas states, of which fundamental understanding is currently lacking.

2 Methodology

2.1 Engine setup

The experiments are conducted on a Ford EcoBoost engine connected to a Horiba transient dynamometer. The engine is a 2-litre, 4-cylinder, GTDI engine with a compression ratio of 9.3:1 and twin independent variable cam timing, which is a representative of modern downsized SI engines. Engine coolant temperature was controlled by a coolant conditioning system. Intake air temperature was controlled by a water-to-air intercooler. The engine was controlled and monitored by a *Motec MI42 ECU* with open, developmental access. A custom firmware was developed to control the engine’s subsystems such as ignition, fuel injection, boost pressure control, camshaft phasers and throttle body. To keep the engine’s production configuration, all stock subsystems were used and no cylinders were deactivated. The calibration data provided by the engine manufacturer were implemented in the ECU. The engine was fitted with four Kistler 6125C piezoelectric pressure transducers. A high-speed data acquisition system using National Instruments hardware was developed for cylinder pressure measurement at 0.1 crank angle degree (CAD) resolution. Online combustion analysis was implemented with an in-house LabVIEW Visual Instrument, which enabled real time monitoring of mass fraction burned, cycle-to-cycle variation, and knock intensity.

Table 2 Engine specifications.

Engine type	Inline 4-cylinder, gasoline turbo direct injection (GTDI)
Displacement volume	1999 cc
Stroke and bore	83.1mm & 87.5 mm
Compression ratio	9.3: 1
Maximum boost	2.1bar (absolute) @ 5000RPM
Valvetrain	Twin independent variable valve cams (intake and exhaust) with 50° adjustment
Fuel injection	7-hole direct injector, variable injection timing and fuel pressure up to 15 MPa

2.2 Method for determining K

In our previous work, two types of methods were identified for determining K in the OI model [25]. One is termed “Regression method” which is based on regression analysis of anti-knock performance of a set of test fuels; the other is termed “PRF method” which is based on matching anti-knock performance of a PRF and the test fuel. The “PRF method” was recommended for its rigor and accuracy for K determination and is used in this work. This method considers that if two fuels demonstrate the same knock resistance at a given engine operation condition (a combination of engine load, speed and air-fuel ratio), the octane index of the two fuels should be equal at this condition. Since PRFs have the same RON and MON ($S = 0$), their OI is invariant with K (Eq. 2) and always equal to its RON and MON. Using this idea, the OI of a sensitive fuel can be determined by matching its knock resistance to that of a PRF, for example, by matching the knock-limited CA50 (crank angle location of 50% fuel burned). The K can then be determined with Eq. 3 using the RON and S of the test fuel (RON_{test} and S_{test} , respectively) and OI at this condition ($OI = RON_{PRF}$).

$$K = \frac{RON_{test} - OI}{S_{test}} = \frac{RON_{test} - RON_{PRF}}{S_{test}} \quad Eq. 3$$

The PRF method was first proposed by Mittal et al. [17] and later adopted by several authors [24, 25]. In these studies, calibration curves for OI were first developed from testing a set of PRFs at a certain octane number interval. K was then determined from Eq. 3 by testing a sensitive fuel and interpolating the result between these curves. Accuracy of this method depends on the octane number resolution between these calibration curves, which is generally several octane numbers. K thus determined can have significant uncertainty. To address this issue, this work develops an online fuel blending system which blends iso-octane and n-heptane in real time to produce a PRF of the needed composition that matches the OI of the test fuel. Details of the fuel blending system are provided in the next section.

A US EPA Tier III 91.6-RON certification gasoline (from Gage Products, Ferndale, MI, USA) was used as the test fuel in this work. The fuel properties are listed in Table 3 along with that of PRFs. The certification fuel has a RON of 91.6 and a MON of 83.4 and contains 9.85% ethanol by volume, representative of a U.S. regular grade E10 gasoline.

Table 3 Properties of the Tier 3 certification gasoline and Primary Reference Fuels (PRFs) used in this study.

	US EPA Tier III 91.6-RON Certification Gasoline	PRF (0-100)
RON	91.6	0 – 100
MON	83.4	0 – 100

S	8.2	0
H/C (mole/mole)	2.026	2.286 – 2.250
O/C (mole/mole)	0.033	0
Ethanol (vol. %)	9.85	0
Net heating value (MJ/kg fuel)	41.67	44.57 – 44.31
HoV (MJ/kg fuel @25°C)	0.41 ^[26]	0.37 – 0.31 ^[27]
Stoichiometric A/F ratio (mass)	14.05	15.10 – 15.05

2.3 Online PRF blending system

2.3.1 Design of PRF blending system

Figure 1 shows a schematic of the PRF blending system. The system used two Coriolis mass flow controllers (MFCs) to control the flow rates of iso-octane and n-heptane. A static mixer was used to facilitate mixing of the two fuel streams. The PRF mixture was delivered at a constant pressure of 5.7 bar to the engine DI pump, the same pressure as that delivering the certification gasoline. The control logic is to first set the total flow rate per the engine operating condition and then set the individual flow rates of iso-octane and n-heptane at the MFCs per the desired PRF number (or octane index, which are the same for PRFs). Because the fuel flow rate demanded by the engine is a function of manifold air pressure (MAP) and engine speed, a look-up table was created to determine the total flow rate using measured MAP and engine speed.

Figure 1 Schematic of the online fuel blending system (ic8 = iso-octane, nc7 = n-heptane).

2.3.2 Verification of performance

Accuracy and dynamic response of the blending system were examined using offline and online tests.

2.3.2.1 Accuracy of the blending system

Offline tests, where the blending system was disconnected from the engine, were conducted to examine whether the produced PRF compositions matched the commanded value. Two mixture properties, density and octane number, were tested to this purpose.

In the density measurement, due to the very similar densities of iso-octane (688.02 kg/m³ at 25°C and 1 atm) and n-heptane (679.72 kg/m³), toluene was used to replace n-heptane for its much different density (862.37 kg/m³). The blending system first mixed toluene and iso-octane at different volumetric fractions. The densities of the prepared mixtures were calculated using REFPROP [28] and measured with a volumetric flask on a weight scale. Comparison of the densities from the two methods showed a discrepancy less than 0.1% (Table 4), equivalent to less than 0.1 octane number if iso-octane/n-heptane mixtures were used. This uncertainty is well below the smallest tolerance allowed for octane number measurements, which is 0.2 octane number for repeatability at 90-100 ON [4, 5].

Table 4 Density of iso-octane/toluene mixtures.

Toluene concentration (% vol.)	25	50	75
Density from REFPROP (kg / m³)	729.32	772.72	816.13
Density from measurement (kg / m³)	728.66	773.01	816.62
Relative error (%)	0.09	0.03	0.06

In the octane number test, the blending system mixed iso-octane and n-heptane and prepared PRFs with octane number of 87, 89 and 91. The RONs of these mixtures were then measured in a CFR engine at the University of Melbourne following ASTM D2699 procedures. The CFR engine has been used in our recent octane blending studies [29-31]. The results are shown in Table 5. The difference in octane number is less than or equal to 0.2. This difference is greater than that from the density measurement because the octane number measurement includes the uncertainty of both the fuel blending system and the CFR engine. For K determination, a difference of 0.2 octane number will result in a difference of 0.024 in K value for the 91.6-RON certification gasoline with an octane sensitivity of 8.2, which is deemed sufficient for the present study.

Table 5 Comparison of the targeted octane numbers vs. measured octane numbers by CFR engine.

Commanded PRF number	87	89	91
Octane number measured on the CFR engine	87.1	89.2	91.2

2.3.2.2 Dynamic response of the blending system to engine operation

An online test was conducted to assess the dynamic fitness of the fuel blending system for engine experiments. In this test, the blending system supplied PRF mixtures to the DI pump when the engine was running. Upon receiving a command for a new PRF number, the blending system adjusted itself automatically to produce the PRF of the required composition while maintaining the total flow rate demanded by the engine. The PRF number was changed stepwise from 98 to 85 at a fixed total flow rate of 15 kg/hr, corresponding to that required by the engine at a speed of 3000 RPM and a load of 6 bar brake mean effective pressure (BMEP). As shown in Figure 2a and Figure 2b, the flow rates of iso-octane and n-heptane responded promptly to the commands and reached the set points within ~20 seconds, leading to smooth transitions between PRF numbers. The total flow rate and the fuel pressure downstream of the blending system are shown in Figure 2c. The fuel flow rate was stabilized at 15 kg/hr except for the transition points where the total flow rate increased by 0.2 kg/hr. However, this small change was damped by the back-pressure regulator, and as a result, the fuel pressure upstream of the DI pump was not affected, nor was the engine performance. This test therefore verified the suitability of the online fuel blending system for providing a controllable PRF mixture during engine testing.

Figure 2 Response of the online fuel blending system to PRF number changes at 3000 RPM and 6 bar BMEP. (a) Fuel flow rates of iso-octane and n-heptane, (b) PRF numbers of the mixture (calculated from the flow rates) and (c) total flow rate and fuel pressure.

2.4 Engine operation and knock detection

The K determination was conducted at “trace knock” or “borderline knock” conditions, which is a transition condition between normal, knock-free combustion and continuous knocking. The trace knock condition was determined by both audible signals measured by a microphone installed on the engine block and in-cylinder pressure oscillations. For the latter, power-spectral density analysis was conducted to the measured cylinder pressures which showed a characteristic frequency of 6.4 kHz for the first acoustic mode of engine knock. A bandpass filter of 3 – 10 kHz was then applied, and the peak-to-peak variation of the filtered pressures was used to determine the knock intensity. A cycle was deemed to be knocking if the peak-to-peak oscillation exceeded a threshold value, which was set at 0.5 bar at 1000 – 3000 RPM and linearly increased to 1 bar at 5000 RPM due to stronger background noise at high engine speeds [32]. This threshold setting does not affect the K determination using the PRF method, as observed previously [24]. An operating condition was defined to be trace knocking when the oscillation of 5% of every 300 cycles exceeded the threshold.

The experiment conditions were selected from the engine operation map at normal temperature and high temperature conditions (Table 6). At the normal temperature condition, the intake manifold temperature and coolant temperature were held at 43°C and 90°C, respectively, which represented the engine’s thermal condition during standard EPA drive cycle tests. At the high temperature condition, the intake manifold temperature and coolant temperature were increased to 70°C and 105°C, respectively, which were used to simulate the engine’s condition in the SAE J2807 towing tests [33]. Figure 3 shows the operating conditions at both temperatures. For the normal temperature test, both knock-limited conditions and over-advanced conditions were tested which aimed to include K values at part load where the engine could be knock-limited with higher compression ratio or lower octane fuels. The *knock-limited condition* is where the CA50 is retarded from the maximum brake torque (MBT) timing, and the *over-advanced condition* is where the CA50 is advanced beyond the MBT timing until knock starts to occur.

Table 6 Engine operating conditions.

	Normal T test	High T test
Engine speed (RPM)	1000 – 5000	2000 – 5000
Engine BMEP (bar)	6 – 18	6 – 14
Intake manifold temperature (°C)	43	70
Coolant temperature (°C)	90	105

Figure 3 Engine operating conditions for K measurement at (a) normal and (b) high temperature conditions. The solid symbols represent knock-limited conditions with CA50 retarded from the MBT timing. The hollow symbols are for over-advanced conditions with CA50 advanced from the MBT timing.

2.5 Experimental procedures

The trace knock combustion in this work was systematically approached by applying the following operating limits:

1. CA50 is between 0 and 30 °CA after TDC;
2. The exhaust temperature before the turbine is less than 900 °C;
3. Lambda is greater than 0.75;
4. The octane index is no greater than 100.

For a given engine speed, the load sweep started at 6 bar BMEP or the load with trace knock occurring at CA50 = 0°CA, whichever had a later CA50. The load was then increased at a step of 2 bar BMEP, and the CA50 was adjusted until the trace knock condition was reached. The increasing knock propensity was controlled by retarding CA50, and if needed also enriching the combustion mixture, subject to the limits specified above. Fuel enrichment was also used to mitigate the exhaust temperature to protect the turbine, particularly at high speed and high load conditions. With the PRF method, the highest OI was limited to 100. As a result, maximum load conditions where the OI of the 91.6-RON certification fuel exceeded 100 were not tested.

At each speed-load point, the OI and K were determined by matching the BMEP and CA50 of the 91.6-RON certification gasoline with a PRF using the following procedures:

1. The 91.6-RON certification gasoline was first tested with lambda at 1, and the spark timing was advanced until trace knock emerged. Fuel enrichment was applied if the CA50 approached 30°CA aTDC or the exhaust temperature approached 900 °C. The resultant knock-limited CA50 is denoted as CA50_{test}.

2. Fuel was switched from the gasoline to the PRF system. To avoid excessive knocking, PRF100 (neat iso-octane) was first supplied. The throttle position and lambda were adjusted to match the BMEP and lambda of the gasoline.
3. Spark timing was advanced to make $CA50_{PRF100}$ equal $CA50_{test}$ while maintaining a constant BMEP and lambda.
4. The PRF number was then reduced from 100 while keeping $CA50_{PRF}$ equal to $CA50_{test}$ until trace knock was detected.
5. The obtained PRF number determined the OI of the 91.6-RON certification gasoline at this condition and from which K was calculated with Eq. 3.

2.6 Calculation of end gas temperature

The end gas temperature was determined by iterative simulations using GT-Power software [34]. First, the mass fraction burned (MFB) profile was estimated using the Rassweiler-Withrow method with the measured cylinder pressure profile [35]. A full engine model including detailed engine geometry was then used to derive in-cylinder conditions such as the wall temperature, residual gas fraction and fuel vaporization profile, using a semi-predictive combustion sub-model. The results further fed to a reverse run model to reproduce the cylinder pressure history and from which to determine a more accurate MFB profile. The obtained burn rate was finally used in the full engine model to produce the unburned gas temperatures.

The GT-Power simulation does not consider fuel chemistry and thus is unable to simulate the low-temperature or intermediate-temperature heat release (LTHR or ITHR) during end gas compression. Recent studies showed that these heat releases could affect the pressure-temperature trajectory [36] in SI combustion, especially when using PRFs as the fuel. However, the impact of these heat releases on the end gas temperature is considered to be minor in this work. This can be partially verified by the results in Ref. [36] which measured the pre-spark heat releases for a 99 RON gasoline (containing 80 vol.% saturates and 20 vol.% aromatics) in a similar GTDI engine. At 2000 RPM and 20 bar IMEP, the pre-spark heat release was observed to increase with intake temperature but below 70°C none was detected. Given the similar engine setup and a less paraffinic fuel used in this work, it is reasonable to estimate that the 92 RON E10 gasoline should produce less pre-ignition heat release at 2000 RPM, 16 bar BMEP with an intake temperature of 43°C. The likelihood to produce such heat release at other conditions should be even lower for the higher K values. With further compression by the flame, the end gas reactions might produce detectable amount of heat release. Estimation of such heat release will require a gasoline surrogate and a chemical kinetic model that is validated for engine applications, which, however, based on our recent work [37] still requires major efforts for development. Therefore, GT-Power simulation without considering the end gas chemistry was used in the present study.

End gas temperatures were investigated for 31 test conditions in the EcoBoost engine and for 2 test conditions in the CFR engine. The CFR engine tests were conducted at the standard RON and MON conditions with a toluene reference fuel, TRF91-45. The fuel contains 45% toluene, 34.7% iso-octane, and 20.3% n-heptane (all by volume) and has similar octane numbers to that of the 91.6-RON certification fuel, as shown Table 7. Including the CFR data enables testing of whether K is related to end gas conditions in some universal way, independent of the fuel and engine used, as is hypothesised [21].

Table 7 Octane numbers of TRF91-45 and EPA Tier III 91.6-RON certification gasoline.

	RON	MON	S
TRF91-45	91.2	83.6	7.6
Certification gasoline	91.6	83.4	8.2

3 Results

3.1 Repeatability tests

To ensure the consistency of K measurement, reference experiments were repeated regularly at 1500 RPM, 6.5 bar BMEP and normal temperature conditions. Figure 4 shows a set of repeatability tests taken over several days of experimentation. The observed confidence interval of 0.025 corresponds to an uncertainty of 1.2% relative to the total measured range of K, from -1.0 to 1.1.

Figure 4 Measured K values from repeatability tests at 1500 RPM, 6.5 bar BMEP and normal temperature conditions.

3.2 Normal temperature results

The results of K and OI for load sweeps at 1000-3000 RPM at normal temperature conditions are plotted in Figure 5. The K values show a consistent and strong decreasing trend with the engine load, as is known in the literature [17, 21, 25, 38]. The K values are well above zero at part-load conditions and reach +0.6 at the lowest loads, indicating that the MON is somewhat more closely related to the anti-knock quality at the condition than the RON. However, these low-load conditions are not all knock-limited for the 91.6-RON certification gasoline in the CR 9.3:1 engine (as indicated by the open markers). The engine becomes knock limited when K is approximately 0.2 or lower across this speed range. At a given BMEP, the promoting effect of engine speed on K is evident, which is also consistent with what has been found in previous studies [21, 22, 25]. The OI values show the same trend as K. The fuel is less knock-prone at higher engine speeds, primarily due to the reduced time available for autoignition. Corresponding to the common K of 0.2 when the combustion starts to be knock-limited, the OI where the combustion starts to retard from the MBT (solid symbols) are almost identical for all speeds, which are approximately 90 for the 92 RON fuel. The proximity of this OI and the RON indicates that the condition where the engine starts to be knock-limited is close to that in the RON test, which is in general agreement with the argument that the RON is a better predictor of anti-knock performance than MON in modern engines.

Figure 5 Measured a) K value and b) OI at 1000–3000 RPM and normal temperature conditions for the 91.6-RON certification gasoline. The solid symbols are knock-limited and the hollow symbols are over-advanced.

Detailed operating conditions for some of these K measurements are provided in Figure 6. Combustion retard and fuel enrichment were used to ensure that the operating limits discussed in Section 2.5 were not exceeded. As the engine load increased, combustion phasing was consistently retarded for knock control. Lower speeds required more retard, for example, at 1250 RPM, fuel enrichment was required at 12 bar BMEP to prevent the CA50 being retarded beyond 30° aTDC, whereas at 2500 and 3000 RPM, CA50 did not reach 30° aTDC until nearly 16 bar BMEP. However, for the latter two speeds, the exhaust temperature reached the limit of 900°C at 14 bar BMEP; therefore, fuel enrichment was used above 14 bar BMEP to control both exhaust temperature

and combustion phasing. At 18 bar BMEP, the combustion at 2500 RPM requires an even richer mixture than at 3000 RPM because of a more retarded CA50.

Figure 6 (a) Exhaust lambda, (b) CA50 and (c) exhaust temperature from load sweeps at 1250, 2000 and 3000 RPM and normal temperature conditions for the 91.6-RON certification gasoline. The color bands indicate the operating limit of these parameters. The solid symbols are knock-limited and the hollow symbols are over-advanced. The exhaust temperatures at 1250 RPM are below 700°C and therefore not shown.

Results of K and OI at 4000 and 5000 RPM are plotted in Figure 7, together with that of 3000 RPM for reference. Compared with the K at 1000-3000 RPM, the effect of engine speed is diminished, and the K is only different by approximately 0.1 between the two speeds. The K values at 4000-5000 RPM are also lower than that at 3000 RPM, showing an opposite effect to that at 1000-3000 RPM. In addition, the K value at which the combustion starts to be knock limited is higher, which is close to 0.5 at 8 bar BMEP, showing higher relevance of MON at high speed, medium load conditions.

Figure 7 Measured K and OI at 3000 – 5000 RPM and normal temperature conditions for the 91.6-RON certification gasoline. The solid symbols are knock-limited and the hollow symbols are over-advanced.

Fuel enrichment was intensively used at these conditions as shown in Figure 8a. However, in this case fuel enrichment was used not due to the CA50 reaching the retard limit (Figure 8b), but due to the high exhaust temperature associated with high engine speed (Figure 8c).

Figure 8 a) Exhaust lambda, b) CA50 and c) exhaust temperature of load sweeps at 4000 and 5000 RPM and normal temperature conditions for the 91.6-RON certification gasoline. The color bands indicate the operating limit of these parameters. The solid symbols are knock-limited and the hollow symbols are over-advanced.

The non-monotonic variation of K with engine speed appears to be related to the end-gas temperature. Figure 9 shows the simulated end-gas temperatures from 2000 RPM to 5000 RPM at a constant load (12 bar BMEP). To better indicate the end gas condition, the end gas temperature is plotted as a function of mass fraction burned. During the main combustion (CA20 – CA80), the end gas temperature is lowest for the 2000 RPM case due to the most retarded CA50 (27.4 CAD aTDC, in comparison with the CA50 at other speeds shown in Figure 6b and Figure 8b), which corresponds to the lowest K of this case. The end gas temperature is highest at 3000 RPM, where K also peaks, and then decreases again as engine speed increases to 5000 RPM, mainly due to the strong fuel enrichment.

Figure 9 Simulated unburned gas temperatures of the 91.6-RON certification gasoline as a function of the mass fraction burned (MFB) at 2000 – 5000 RPM, 12 bar BMEP and normal temperature conditions.

With the K values measured over a wide range of operating conditions, a contour map can be generated over the engine speed-load map for K (Figure 10). The red line represents the knock-limited boundary, above which the CA50 is retarded from the MBT timing, with associated reduction in fuel efficiency, and below which the CA50 is over-advanced. Figure 10 shows that K can be positive at knock-limited conditions, especially at high engine speeds, but for the majority of the area above the knock-limited line K is zero or negative. It should be noted that all knock-limited conditions here are referenced to the CR 9.3:1 engine and the 91.6-RON certification gasoline. The over-advanced conditions can become knock limited if a higher compression ratio engine or a lower octane number fuel is used. Proposals that MON specifications should be lowered or even removed for market gasolines should therefore be carefully evaluated. Care should also be taken with proposals that would specify a minimum S and would indirectly set a maximum MON value that is too low.

Figure 10 K map for normal temperature operation. The red line delineates knock-limited (above) and over-advanced (below) conditions.

3.3 High temperature results

Figure 11 and Figure 12 show the results for K and OI at the high operation temperature, along with those at the normal temperature. Similar to the normal temperature case, K decreases with engine load across the speed range and is insensitive to engine speed at 4000-5000 RPM. Due to the elevated temperature, the operation becomes knock-limited at lower BMEPs, and the knock-limited K moves to more positive ranges. For example, the knock-limited K can be greater than 1, i.e. beyond MON, at medium loads. Correspondingly, the fuel's knock resistance drops to a level where the OI is as low as approximately 82.

Figure 11 Comparison between the measured a) K and b) OI for the 91.6-RON certification gasoline at 2000-3000 RPM at high and normal temperature conditions. The solid symbols are knock-limited and the hollow symbols are over-advanced.

Figure 12 Comparison between the measured K and OI for the 91.6-RON certification gasoline at 4000-5000 RPM at high and normal temperature conditions. The solid symbols are knock-limited and the hollow symbols are over-advanced.

Comparing the two operation temperature cases, K values at high temperature conditions show a steeper drop with engine load, causing the two curves to cross at one point. At the lower-load side of the crossover, K is higher with the high temperature, which is consistent with the general understanding of the temperature impact on K. However, at higher loads, K becomes lower for the high temperature case, which can be explained as follows. With the high charge temperature, higher intake pressure is required to compensate for the reduced charge density to produce the same BMEP. Since increasing temperature and pressure both promote knock, more combustion retard and/or fuel enrichment are required to suppress knock. Both factors lead to a lower end gas temperature and consequently a lower K value. The same effect should also take place at lower loads (to the left of the crossover) but apparently is not as significant as at higher loads. Figure 13 shows an example for this. At 2000 RPM and 8 bar BMEP, the end gas temperature of the high temperature case is consistently higher than the normal temperature case, despite the more retarded combustion timing, and therefore causes higher K. After the crossover, at 12 bar BMEP, the more retarded combustion phasing of the high temperature case now produces lower end gas temperatures during 10 to 35°CA aTDC, which is the most critical duration where knock could occur due to the flame compression. The lower end gas temperature during this process therefore leads to a lower K for the high temperature case. The relation between K and end gas temperature will be further discussed in the next section.

Figure 13 End gas temperatures of the 91.6-RON certification gasoline at two operating conditions (8 and 12 bar BMEP, 2000 rpm) with normal and high temperatures.

The K map for the high temperature condition is presented in Figure 14. Comparing with Figure 10, this map covers a smaller load space but the K values are more positive. The effect of engine speed on K appears less pronounced as indicated by the flatter contour across the speed range. On the other hand, the effect of BMEP on K is stronger, as evidenced by more densely distributed contour lines.

Figure 14 K map for high temperature operation. The red line delineates knock-limited (above) and over-advanced (below) conditions.

3.4 End-gas states and their correlation with K

Engine knock is fundamentally determined by the condition of unburned gases ahead of the flame, and the K value has been suggested to reflect these conditions [23, 39]. Several studies have correlated end-gas states

and K [23, 24, 40], mostly at high load conditions. With the large number of K values obtained in this work, the relationship between K and end-gas states is investigated.

3.4.1 Temperature-pressure trajectory

Several studies have investigated the pressure-temperature trajectory of unburned gases to understand the fundamentals of K [22, 23, 38, 40, 41]. These studies generally concluded that K decreases with lower charge temperature and/or higher cylinder pressure. These trends are also observed in this study. As shown in Figure 15, increasing the engine loads at 2000 RPM shifts the T-P trajectory to lower temperatures since less compression is required to reach a given pressure; correspondingly, K consistently decreases at higher loads.

Figure 15 Unburned gas T-P trajectory of the 91.6-RON certification for a load sweep at 2000 RPM and normal temperature conditions.

However, the T-P trajectories are remarkably insensitive to engine speed. As shown in Figure 16, the T-P trajectories from 2000 to 4000 RPM almost overlap at a given load, and the 5000 RPM curve shows a slight deviation only due to fuel enrichment. This finding is consistent with the results in [42] which reported that changing engine speed did not significantly alter the T-P trajectory but only affected the time elapsed at a certain temperature and pressure.

Figure 16 Unburned gas T-P trajectory of the 91.6-RON certification gasoline for an engine speed sweep at 10 bar BMEP and normal temperature conditions.

Another method to explore the fundamentals of K is to correlate K with a single state on the T-P trajectory. For example, T_{comp15} is the charge temperature when the cylinder pressure reaches 15 bar, and has been found to correlate well with K in HCCI engines [39, 43] but less well in SI engines [23, 38]. Figure 17 shows K plotted against T_{comp15} , including those from the standard RON and MON tests (with TRF91-45) for which K is 0 and 1, respectively. There is a reasonable, linear correlation ($R^2 = 0.746$) between T_{comp15} and K , with the two points from the CFR engine falling within the dataset.

Figure 17 Correlation of K and T_{comp15} for the conditions tested on the EcoBoost engine (91.6-RON certification gasoline) and the CFR engine octane tests (TRF91). The shape of the marker represents the engine speed and the marker color represents the BMEP.

3.4.2 Relationship between K and unburned gas temperature

Further efforts are now spent considering other unburned gas states that could better correlate with K . This considers that T_{comp15} is only one state along the polytropic compression from the inlet value closure (IVC). However, in SI engines, autoignition of the end gas is directly driven by the flame compression, and a state before spark discharge such as T_{comp15} does not capture this flame-induced compression effect. Rather, if K has some physical basis in engine autoignition, it should correlate with the thermodynamic states of the end gas at some point close to the onset of autoignition.

Linear regression for K and unburned gas temperatures during the combustion is therefore applied. Figure 18 summarizes the R^2 of linear correlation at different points in the engine cycle. At the spark timing, the temperature appears uncorrelated with K , whereas an increasingly better correlation is observed until CA70. The R^2 is nearly 0.89 from CA60 to CA90, indicating that the end-gas temperature in the later stage of combustion is more relevant to K .

Figure 18 R^2 for the linear correlation of K and the unburned gas temperatures from the EcoBoost engine tests (91.6-RON certification gasoline) and the CFR engine octane tests (TRF91) at different mass fractions burned.

The best correlation with K is with the end-gas temperature at CA70, as shown in Figure . The two points from the CFR engine using TRF91-45 also follow the trendline, suggesting a possible independence of this correlation to the engine design and fuel.

The strong correlation of K with end-gas temperatures from CA60 to CA80 can be attributed to two main factors. First, end-gas autoignition is primarily driven by the oxidation chemistry at low- to intermediate-temperatures where the temperature is the dominant parameter that controls the process. If this is the case, knock should then first appear late in any burn that commences close to knock limited spark timing since this is the hottest part of the cycle and has the most direct impact on knock. Indeed, previous studies have reported that knock occurred near CA60 to CA80 in SI engines [44-46]. Secondly, end-gas temperature at CA60 – CA80 incorporates all thermochemical effects that occur early in the cycle on knock. For example, engine speed affects the time of heat transfer throughout the cycle, but the cumulative effect on knock cannot be captured by temperatures early in the cycle, rather it will manifest in the end-gas temperature in the later phase.

Figure 19 Correlation of K and the unburned gas temperatures at CA70 from the EcoBoost engine tests (91.6- RON certification gasoline) and the CFR engine octane tests (TRF91). The shape of the marker represents the engine speed and the marker color stands for the BMEP.

It is also interesting to note from Figure 18 that K and the unburned gas temperature at spark timing are nearly independent, with a R^2 approaching zero. The reason behind this can be illustrated by the selected cases shown in Figure , where a lower temperature at the spark timing can lead to either a higher temperature at CA50 (e.g. 10 bar vs 14 bar BMEP cases) or a lower temperature at CA50 (e.g. 18 bar vs. 14 bar BMEP cases). In the former, the higher CA50 temperature is mainly due to the more advanced combustion phasing, whereas in the latter the lower CA50 temperature is primarily due to the stronger fuel enrichment. Variation of combustion retard and fuel enrichment in the engine experiments therefore complicates the connection between the spark timing temperature and those at later stage of combustion, leading to the poor correlation between K and spark timing temperatures.

Figure 20 Simulated unburned gas temperatures of the 91.6-certification gasoline at selected loads, 3000 RPM and normal temperature conditions, showing how the temperature variation at spark timing do not infer that later in the burn.

3.4.3 Relationship between K and cylinder pressure

Pressure is the other major parameter affecting engine autoignition. The R^2 for linear regression of K and cylinder pressure is summarized in Figure 19 as a function of the burned mass fraction. K correlates best with the cylinder pressure at spark timing, but the correlation with pressures becomes consistently worse at later stages of the burn.

Figure 19 R^2 for the linear correlation of K and cylinder pressures from the EcoBoost engine tests (91.6-RON certification gasoline) and the CFR engine octane tests (TRF91) at different mass fractions burnt.

The correlation between K and the cylinder pressure at spark timing is shown in Figure 20. This good correlation is likely because the pressure at spark timing is related to the end-gas temperature during the polytropic compression from IVC, as evidenced by a similar R^2 between T_{comp15} and K (Figure 17). The in-cylinder pressure during the burn then increasingly diverges in its correlation with the end-gas temperature, and consequently the correlation of K with the in-cylinder pressure falls, as Figure 21 showed. Thus, the opposing trends in Figure 18 and Figure 21 is to be expected.

Figure 20 Correlation of K and cylinder pressures at spark ignition from the EcoBoost engine tests (91.6-RON certification gasoline) and the CFR engine octane tests (TRF91). The shape of the marker represents engine speed and the marker color stands for BMEP.

4 Conclusions

This work examined how the *K factor* defined in the Octane Index model varied across a wide range of operating conditions in a modern, 4-cylinder, 2L, turbocharged, gasoline direct injection engine. *K* quantifies the relative significance of RON and MON. For example, when *K* is less than 0.5, knock propensity is better described by RON than MON. The main findings of this paper are summarized as follows.

- A novel, real-time and controllable Primary Reference Fuel (PRF) blending system was first developed to facilitate determination of *K* by matching the knock onset of the 91.6-RON certification fuel with that of a PRF at the same engine operating conditions. *K* was measured at 55 engine operating conditions with normal and high intake air and coolant temperatures and ranged from -1.0 to +1.1 with an uncertainty ± 0.025 . This covered nearly all conditions where the engine could be knock-limited and differed from previous efforts which have mostly focused on high-load conditions.
- Under knock-limited conditions, *K* was mostly negative with normal temperature operation but was mostly positive with higher temperature operation. Indeed, the highest observed knock-limited *K* was above 1. Whilst the RON remained the more important of the two octane numbers overall, this result demonstrated the relevance of the MON to modern engines under some conditions.
- *K* was found to decrease with increasing BMEP at all conditions studied. The impact of other engine operating parameters, particularly the engine speed and air/coolant temperature, was less consistent. This was likely because the end gas temperature did not change monotonically with changes in the other operating parameters. Note that the engine experiments were performed with the factory calibration (e.g. variable camshaft timing), and with exhaust temperature limited by enrichment, in order to obtain *K* results which are realistic for practical applications.
- Simulations of this modern engine enabled examination of the relationship between the measured *K* variations and the simulated, in-cylinder, end gas conditions, with the strongest observed correlation being between *K* and the unburned gas temperature in the later stages of combustion (CA60-CA80). Since knock should first appear late in any burn that commences close to the knock-limited spark timing, and the unburnt gas temperature should be the primary contributor to the fuel's reactivity, this observed correlation has a sound physical basis.
- Simulations of the in-cylinder, end gas conditions during the RON and MON tests of a Toluene Reference Fuel (TRF) in the CFR engine demonstrated a consistent correlation between *K* and the late stage, unburned gas temperature in the GTDI engine. This suggests that the main causes of *K* variations in the modern engine and the CFR engine are shared, supporting the utility of this *K factor* method.

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5 Abbreviations

AKI	Anti-knock index
aTDC	After top dead centre
BMEP	Brake mean effective pressure
bTDC	Before top dead centre
C_{Axx}	Crank angle of xx% fuel burned

CFR	Cooperative Fuel Research
ECU	Engine control unit
GTDI	Gasoline turbocharged direct injection
HCCI	Homogeneous charge compression ignition
HoV	Heat of vaporization
IMEP	Indicated mean effective pressure
KI	Knock intensity
KLSA	knock-limited spark advance
LTHR	Low-temperature heat release
MAP	Manifold air pressure
MBT	Maximum brake torque
MFC	Mass flow controller
MON	Motor octane number
OI	Octane index
ON	Octane number
PRF	Primary reference fuel
RON	Research octane number
RPM	Revolution per minute
S	Octane sensitivity
SI	Spark ignition
T_{comp15}	Unburned gas temperature at compression pressure of 15 bar
TDC	Top dead centre
VVT	Variable valve timing