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# Relating the octane numbers of fuels to ignition delay times measured in an ignition quality tester (IQT)

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## HIGHLIGHTS

- A methodology for estimating the RON and the MON of fuels using an IQT is presented.
- Estimated RON and MON are in good agreement with values obtained from standard tests.
- The DCN of PRFs, TRFs, TPRFs FACE and certification gasolines are reported.
- Correlation between DCN and RON is provided.

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## ABSTRACT

A methodology for estimating the octane index (OI), the research octane number (RON) and the motor octane number (MON) using ignition delay times from a constant volume combustion chamber with liquid fuel injection is proposed by adopting an ignition quality tester. A baseline data of ignition delay times were determined using an ignition quality tester at a charge pressure of 21.3 bar between 770 and 850 K and an equivalence ratio of 0.7 for various primary reference fuels (PRFs, mixtures of iso-octane and *n*-heptane). Our methodology was developed using ignition delay times for toluene reference fuels (mixtures of toluene and *n*-heptane). A correlation between the OI and the ignition delay time at the initial charge temperature enabled the OI of non-PRFs to be predicted at specified temperatures. The methodology was validated using ignition delay times for toluene primary reference fuels (ternary mixtures of toluene, iso-octane, and *n*-heptane), fuels for advanced combustion engines (FACE) gasolines, and certification gasolines. Using this methodology, the RON, the MON, and the octane sensitivity were estimated in agreement with values obtained from standard test methods. A correlation between derived cetane number and RON is also provided.



## 1. Introduction

Engine knock, an abnormal combustion phenomenon that occurs in internal combustion (IC) engines, limits the thermal efficiency of spark ignition (SI) engines [1]. It is caused by autoignition in hot spots at the unburned end gas ahead of the expanding flame front and depends on pressure and temperature evolution in the end gas as well as on the anti-knock quality of the fuel. The autoignition or anti-knock quality of a fuel is measured by the research octane number (RON) and the motor octane number (MON), which are determined using the standard test methods prescribed by ASTM D2699 and D2700 [2,3], respectively, with a cooperative fuel research (CFR) engine. In these tests, the knock behavior of a fuel is compared to that of primary reference fuels (PRFs), mixtures of iso-octane and *n*-heptane, with known iso-octane volume percentages. The RON (or the MON) of the test fuel can then be related to that of the PRF that matches its knock behavior.

There are, however, differences in the chemical composition and autoignition chemistry of practical fuels and the PRFs that are used to define the octane scale. In addition, the same gasoline may match different PRFs at different operating conditions. For all practical fuels, the RON is higher than the MON because the temperature of an unburned gas is higher at a given pressure under MON than under RON conditions. This is due to the more severe MON testing conditions, which are performed at an intake mixture temperature of 422 K and an engine speed of 900 rpm as compared with RON testing conditions, which are performed at 325 K and

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600 rpm. As a result, in MON testing, the autoignition chemistry of PRFs is dominated by negative temperature coefficient (NTC) behavior [4]. Practical fuels, at similar conditions, however, do not exhibit NTC behavior and therefore demonstrate the anti-knock characteristics of a lower-octane-quality PRF than what was used in RON testing: RON values are higher than MON values [4]. The anti-knock quality of a fuel can best be described by the octane index (OI) [1,5–8], which is defined as

$$\mathrm{OI} = (1-k)\mathrm{RON} + k\mathrm{MON} \tag{1a}$$

$$\mathrm{OI} = \mathrm{RON} - k\mathrm{S} \tag{1b}$$

Here, the weighting factor $k$ is a constant depending on pressure/temperature histories with time in an end gas [1] and engine speed, and is weakly dependent on mixture strength [1,9]; S is the octane sensitivity defined as (RON−MON); and octane index (OI) is the volume percent of iso-octane in the PRF that matches the knock behavior of the fuel at any given condition. By definition, $k = 1$ under MON testing conditions and $k = 0$ under RON testing conditions. If the temperature of an unburned gas for a specified pressure decreases, the $k$ value decreases [1,6]. Sensitivity (S) can be regarded as a measure of the difference in autoignition chemistry of a fuel at the two operating conditions, while $k$ is a measure of how different the operating conditions are between the two tests. The temperature of the unburned bulk gas at 15 bar designated as $T_{\mathrm{comp15}}$ was introduced in [6], and this information was used to establish a given operating condition with respect to the RON test condition.

Empirically, it has been demonstrated that the $k$ value decreases as $T_{\mathrm{comp15}}$ decreases [1,6]. SI engine design has developed to enable higher pressure for a given temperature to achieve better thermal efficiency and power density. So historically, $T_{\mathrm{comp15}}$ has decreased from the value representative of the MON test such that the importance of MON in describing fuel anti-knock quality has decreased [1,9]. In fact, $T_{\mathrm{comp15}}$ in modern engines is even lower than in the RON test condition and $k$ can be negative, and thus for a given RON, a fuel with lower MON has higher OI and is more resistant to knock. Further efforts to improve SI engine efficiency by downsizing and turbocharging are driving the trend towards more negative $k$ values, while old engines and CFR engines have positive $k$ values [9].

Attempts have been made to interpret the RON and the MON of practical fuels in terms of more fundamental measures of autoignition, such as ignition delay time. Bradley et al. [10] showed that ignition delay times of non-PRFs can be deduced reasonably from the OIs measured in a variety of engine tests using the data available on ignition delay times for PRFs. Analogous to the $k$ weighting factor relating OI to RON and MON, they defined the $\kappa$ factor relating the ignition delay times of non-PRFs to those for PRFs under the same conditions. Perez and Boehman [11] measured the ignition delay times in an ignition quality tester (IQT) for 21 surrogate gasoline fuels to find a poor correlation between the measured ignition delay time with the RON and the MON. Kalghatgi et al. [12] suggested that fuels should be rated on a toluene/$n$-heptane scale rather than using PRFs because with toluene/$n$-heptane blends, toluene reference fuels (TRF), the sensitivity will be high and comparable to that of practical fuels. Using the current RON test, a fuel could be assigned a toluene number by the volume percent of toluene in the TRF blend matching the fuel behavior in the RON test. However, it is possible to find a ternary mixture of toluene, iso-octane, and $n$-heptane (toluene/PRF or toluene primary reference fuel (TPRF) blends) that matches both the RON and the MON of a fuel. Kalghatgi et al. [13] developed empirical correlations to predict the RON, the MON, and octane sensitivity for TPRF blends based on experimental RON/MON measurements of such mixtures.

Standard RON and MON tests are time consuming and require strict control of various parameters involved during engine operation. The methodology presented in this paper, which can be a convenient initial screening tool to determine RON and MON, estimates the RON and the MON from a combustion device other than the CFR engine. This methodology was developed using a constant volume combustion chamber with liquid fuel spray injection, which is capable of operating at various temperatures and pressures. For wide applicability of the developed methodology, a constant volume combustion chamber of a standard IQT (Advanced Engine Technology Ltd.) system was adopted, which is used to determine the derived cetane number (DCN) of diesel fuels based on ASTM D6890 [14] at the charge temperature and pressure of 818 ± 30 K and 21.37 ± 0.07 bar, respectively.

The ignition delay time, $\tau_{id}$, was measured as the time between the start of fuel injection and the start of significant heat release; an average of 32 firings were taken. The DCN is related to the ignition delay time in [ms] by the formula $\mathrm{DCN} = 4.46 + (186.6/\tau_{id})$ for ignition delay times between 3.1 and 6.5 ms, which correspond to DCNs between 64 and 33. The KAUST research IQT (KR-IQT) was modified from the standard IQT, which typically has a fixed volume of injected fuel. Since equivalence ratio is an important parameter affecting ignition delay times, we have made modifications to testing methods adopted in this study as described in [15] to include this ratio (details in the next section).

Ignition delay times for fuels in the diesel autoignition range are typically short and thus contain both physical (evaporation and mixing) and chemical (reactive) time contributions. For fuels in the gasoline autoignition range, RON > 60 and DCN < 30 [6], with relatively long ignition delay times, the physical delay may be much shorter than the chemical delay, which is one motivation for using the KR-IQT for determining OI.

Ignition delay times for the fuel mixtures of PRFs were measured first to provide a baseline data set. Ignition delay time data for octane sensitive TRFs were then used to develop a methodology. Fuel mixtures of toluene primary reference fuels (TPRFs), fuels for advanced combustion engines (FACEs), and certification gasolines were used to validate the methodology.

## 2. Experiment

A schematic of the experimental setup is shown in Fig. 1. The apparatus comprises a KR-IQT, a gas supply system, and several data acquisition setups. The KR-IQT is equipped with a constant volume combustion chamber at 0.21 L, filled with an oxidizing medium that can be pressurized up to a maximum of 21.6 bar and heated with an electric heater to temperatures in the range of 670–860 K. A liquid fuel spray is injected into a pressurized and heated oxidizing environment. A pneumatically driven mechanical pump delivers fuel stored in a fuel reservoir to the injector with a single-hole S-type inward opening pintle nozzle [16]. The temperature of the nozzle tip during operation is around 325 K. The injected fuel mass can be regulated by adopting a pneumatically driven variable displacement pump (VDP), which varies displacement of the pump, thereby the volume of fuel injected. This modification was provided by the manufacturer. It uses turnbuckle bolts, which when rotated, change the displacement between the front body and rear body of VDP using a chain system as was shown in Fig. 3 in [15]. The VDP has a limited displacement range, therefore, for a specified charge pressure, there is a limited range of equivalence ratio available depending on the density and oxygen requirement of the fuel. More details on mass calibration for the VDP have been explained in detail in [15,17].

The fuel is injected into the combustion chamber at a pressure of 225 bar [16]. A piezo-electric pressure transducer mounted