



THE FUTURE OF OCTANE TESTING: A LOOK AT THINGS TO COME

Since the spread and popularization of the automobile by Ford Motor Company's Model T, gasoline has become an indispensable necessity for nearly all automobiles. Early in the history of automobiles, researchers had difficulty in defining the grade and efficiency of gasoline without performing numerous experiments through trial and error [1]. One critical characteristic of any gasoline blend was its propensity to knock. Knock is an engine phenomenon associated with an engine producing a knocking noise caused by the autoignition of portions of the unburned air-fuel mixture in an engine chamber. Knock not only limited the maximum work done by the air-fuel mixture in the cylinder, but heavy knock could also result in engine damage. The gasoline and automotive industry converged on the octane testing method as a technique for capturing the antiknock characteristics of a fuel.

In 1920, a coalition of automotive and fuel companies formed the Cooperated Fuel Research (CFR) committee to create a metric to understand a fuel's tendency to knock [1]. The CFR committee eventually settled on the octane number test as a method of characterizing a fuel's antiknock properties. The octane number tests run a fuel in a specialized test engine called the CFR engine, which was designed to measure knock [2]. The compression ratio of the CFR engine is increased until the engine knocks at a certain intensity. That compression ratio is compared to a reference blend of iso-octane and n-heptane. The subsequent percentage of iso-octane in the reference fuel would then be called the octane number.

The CFR committee found that the octane number was highly dependent on the engine operating conditions. The initial test conditions, with an intake temperature of 52 °C and an engine speed of 600 rpm, was deemed the research octane number (RON) and accepted by the American Bureau of Standards in 1929 [1]; yet, in 1932, it was found that the test conditions used to obtain the RON did not correspond to road conditions [3]. The CFR committee changed the test conditions to an engine speed of 900 rpm and intake temperature of 149 °C creating the motor octane number (MON) [4]. Since iso-octane is less likely to autoignite in comparison to n-heptane [5], the RON and MON of a fuel indicate its susceptibility to knock, where higher RON and MON values lead to a lesser proclivity of engine knocking. Both of these test methods have become the standard for determining the octane rating of gasoline to the present day and are now known as test methods ASTM D2699 and ASTM D2700 [3,4].

Yet, since the conception of the RON and MON test methods, there has been controversy concerning the selection of the reference fuel's components. The current reference fuel has been deemed too simple to properly capture the complex chemistry of actual fuels. Additionally, the reference fuel blend for the RON and MON test methods is solely composed of paraffinic components despite the decreasing concentration of these components in actual fuel blends throughout history. The ever-prevalent use of anti-knock additives such as ethanol also adds another layer of

complexity for the determination of RON and MON for fuels.

Furthermore, the CFR engine was designed in accordance with 1928 automobiles; thus, it is salient that advancements in engine technology be considered when comparing the octane number tests to a fuel's antiknock performance in modern engines. For example, the modern passenger engine has an idle speed of approximately 500 to 1000 rpm which encompasses the engine speeds in the RON and MON tests; however, engines are not likely to knock while idling. Instead, engines have shifted to operating at higher speeds, which is made evident through the increasing trend of engine horsepower. Equation 1 shows the relationship between horsepower, torque, and rpm. An increase in engine horsepower will result in an increase in engine speeds, assuming a constant torque.

$$RPM = \frac{HP \times 5252}{Torque} \quad \text{eq. 1}$$

The older Ford Model T had an output of approximately 22 horsepower; however, current passenger vehicles output well over 100 horsepower, such as the Honda Civic at 158-180 horsepower. While not all of this power is utilized in the average driving route, operating conditions that were once considered as harsh have become tame through technological advancements of the engine.

Considering these points, it is vital that the test methods for determining octane numbers be modified to better characterize current fuel potential with respect to modern engine output. These modifications can range from simply changing the policy for obtaining the octane rating to an overhaul of the original testing methods such as a change in the reference fuel and/or a change in the test conditions to better fit current driving conditions.

The current policy for determining the Anti-Knock Index (AKI) in the United States takes the average value of the RON and MON of a given fuel. The AKI is a simplification of the equation for Octane Index (OI) [10], shown below in Equation 2, and assumes the octane appetite, K, of all engines is 0.5.



$$OI = RON - K \times (RON - MON) = RON - K \times S \quad \text{eq. 2}$$

However, the main issue is that multiple studies have shown the current K-value for a wide variety of modern engines to be close to zero or negative [6, 7, 8, 9]. Notably, modern naturally aspirated engines have an average K-value of -0.02 and modern TC/DI engines have an average K-value of -0.3 [10]. These values indicate that the value of K decreases with increasing intake pressure and increases with increasing intake temperature and engine speed [11]. The trend for modern cars indicates that the K-value will become increasingly negative. A negative K-value implies a positive correlation with RON and negative correlation with MON, suggesting that modern fuels are shifting away from the MON causing the RON to have greater importance in determining the anti-knock properties of a fuel. Thus, it is theoretically possible to phase-out the MON and utilize only the RON to classify a fuel's anti-knock properties. The main concern with this change is that the underlying causes of the shift in K-values are not properly ameliorated. According to equation 2, a negative K-value infers that the octane index improves with increasing fuel sensitivity, S, defined as the difference between RON and MON. Hence, it would imply that fuels should be refined to have higher sensitivities. Thus, a redistribution in the weighting of K-values to modify the AKI has been proposed. Through the assessment of the range of K-values for current naturally aspirated (NA) and turbocharged/direct injection (TC/DI) engine models, as shown in Figure 1, the original reference bounds of K from 0 to 1 do not adequately characterize current automobiles.

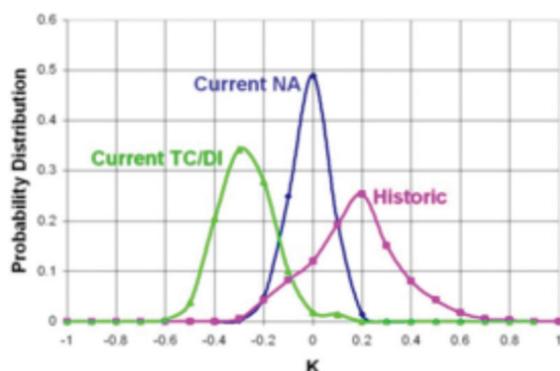


Figure 1. Statistical distribution of K-values for historic, current, and future engines [10].

Instead, K-values could be shifted to -0.75 and 0.25 in order to better incorporate the expected K-values of modern engines and providing a new theoretical reference frame by which the current octane testing methods may be converted to modern standards. While simple, policy changes will at most remain as a superficial adjustment and require other measures to ensure all the underlying flaws have been rectified.

These policy changes alone neither liberate the constraints set forth by the iso-octane/n-heptane reference fuel nor portray the complex chemical interactions of anti-knock additives in gasoline. As previously mentioned, the current components of the reference fuel are strictly paraffinic fuels and do not adequately represent modern fuels. Notably, paraffinic fuels are known to have a negative temperature coefficient where a fuel's anti-knock properties increase with increasing temperature, yet real fuels do not exhibit this behavior [12]. Furthermore, the current reference fuels have a sensitivity of zero meaning the octane index of the reference fuels is independent of changes in the K-value, even though the octane index of commercial fuels depends heavily on the K-value [13]. Thus, researchers such as Kalghatgi et al. [14] have proposed replacing iso-octane with toluene creating a new toluene and n-heptane reference fuel as well as a new metric called the toluene number (TN). The new TN could then be the singular metric utilized to determine the anti-knock quality of gasoline at varying test conditions with greater reliability than the octane index method which requires RON, MON, and the corresponding K-value before calculations are possible.

The introduction of anti-knock additives into gasoline have also begun to push the current octane testing methods beyond its useful bounds. For instance, the anti-knock additive ethanol has an approximate RON of 106-111 and MON of 89-92 [15]. An octane number beyond 100 can only be obtained by an extrapolated octane rating curve or utilizing octane enhancers such as tetra-ethyl lead with the iso-octane reference fuel [14]. Such a method is inherently flawed since the octane number becomes arbitrary as values above 100 do not quantitate relative to the iso-octane reference fuel. As such, the increase in relative bounds by shifting away from iso-octane reference fuels to toluene reference fuels allows for a more accurate and reliable method to interpolate the anti-knock properties of gasoline even with additives. The TN has shown promising results but requires extensive research to create a calibration curve equivalent to that of the RON and MON test methods and, consequently, extensive validation before it can be standardized.

The concept of a metric such as the TN that can be utilized for a variety of test conditions also exposes the stringent requirements of the RON and MON test conditions and its ensuing issues. The current RON and MON tests are framed such that the octane index is equivalent to the RON at $K=0$ and the MON at $K=1$. Yet, current NA and TC/DI engines lay below the original threshold of K-values. It is then possible to reconfigure the RON and MON tests to better imitate modern engines by utilizing the previously mentioned shifted reference frame of K-values (-0.75 and 0.25) to

set the operating conditions for each test, respectively. In practice, the reference frame of -0.75 to 0.25 suggests a modified RON test condition with an intake temperature of 30 °C, engine speed of 900 rpm, and intake air pressure of 1.4 bar; and a modified MON test condition with an intake temperature of 70 °C, engine speed of 1500 rpm, and intake air pressure of 1 bar [16].

These changes allow the RON and MON tests to better bracket the engine speeds, intake pressures, and in-cylinder temperatures of modern engines, hence allowing for better alignment with the autoignition chemistry of modern fuels. All fuels have three distinct autoignition regimes with respect to end-gas temperatures: a low temperature regime below 775 K, a high temperature regime above 900 K, and a transition regime between the high and low regimes. As shown in Figure 2, autoignition chemistry of modern engines tend to occur in the transition regime. Meanwhile, the autoignition in the RON and MON tests occurs in the high temperature regime. The test adjustments allow for a change in the end-gas temperatures in the octane tests, allowing for better alignment with modern engines [17].

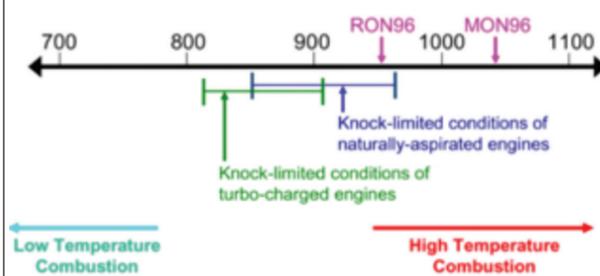


Figure 2. The end-gas temperature spectrum for modern SI engine operation [17].

While changing the engine operating conditions will result in better alignment with end-gas temperatures in modern engines, other changes are necessary as well. For example, the RON and MON tests currently set the air/fuel ratio to maximize knock. Yet, by maximizing knock, knock inducing conditions must be inferred, potentially restricting engine efficiency. As such, it is advisable to change the air/fuel ratio of the RON and MON tests to imitate the stoichiometric ratios used in typical engine operation.

The adoption of the octane number in 1929 has improved engine and fuel efficiency in the United States for the past century; however, the octane test methods have not been modified to match current engine and fuel improvements. As environmental concerns grow increasingly important, countries throughout the world have set forth increasingly stringent regulations on fuel efficiency and emissions. Thus, it is vital that researchers and manufacturers understand the potential of modern fuels and engines. Innovations such as hybrid engines, bio-fuels, and environmentally acceptable gasoline additives have continued to propagate; yet, without an accurate and robust test method for anti-knock properties progress may otherwise stagnate.

References:

- [1] Mittal V., "The Development of the Octane Number Tests and their Impact on Automotive Fuels and American Society," The International Journal for the History of Engineering & Technology, 86:2, 213-227, 2016, DOI: 10.1080/17581206.2016.1223940
- [2] American Society for Testing Materials, 'Standard Test Method for Research Octane Number of Sparkignition Fuel', Annual Book of ASTM Standards, vol. 5.05, 2003, p 19.
- [3] ASTM D2699-19, Standard Test Method for Research Octane Number of Spark-Ignition Engine Fuel, ASTM International, West Conshohocken, PA, 2019, www.astm.org
- [4] ASTM D2700-19, Standard Test Method for Motor Octane

Number of Spark-Ignition Engine Fuel, ASTM International, West Conshohocken, PA, 2019, www.astm.org

- [5] C.K. Westbrook, M. Sjöberg, N.P. Cernansky, "A new chemical kinetic method of determining RON and MON values for single component and multicomponent mixtures of engine fuels," Combustion and Flame, Volume 195, 2018, Pages 50-62, ISSN 0010-2180, <https://doi.org/10.1016/j.combustflame.2018.03.038>.
- [6] Kalghatgi, G., "Fuel Anti-Knock Quality - Part I. Engine Studies," SAE Technical Paper 2001-01-3584, 2001, doi:10.4271/2001-01-3584.
- [7] Kalghatgi, G., Nakata, K., and Mogi, K., "Octane Appetite Studies in Direct Injection Spark Ignition (DISI) Engines," SAE Technical Paper 2005-01-0244, 2005, doi:10.4271/2005-01-0244.
- [8] Kalghatgi, G., "Fuel Anti-Knock Quality- Part II. Vehicle Studies - How Relevant is Motor Octane Number (MON) in Modern Engines?," SAE Technical Paper 2001-01-3585, 2001, doi:10.4271/2001-01-3585.
- [9] Davies, T., Cracknell, R., Lovett, G., Cruff, L. et al., "Fuel Effects in a Boosted DISI Engine," SAE Technical Paper 2011-01-1985, 2011, doi:10.4271/2011-01-1985.
- [10] Mittal, V. and Heywood, J., "The Shift in Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines Over the Last 70 Years," SAE Int. J. Engines 2(2):1-10, 2010, <https://doi.org/10.4271/2009-01-2622>.
- [11] Kieran P. Somers, Roger F. Cracknell, Henry J. Curran, A chemical kinetic interpretation of the octane appetite of modern gasoline engines, Proceedings of the Combustion Institute, Volume 37, Issue 4, 2019, Pages 4857-4864, ISSN 1540-7489, <https://doi.org/10.1016/j.proci.2018.05.123>. (<http://www.sciencedirect.com/science/article/pii/S1540748918301299>)
- [12] Remmert, S., Campbell, S., Cracknell, R., Schuetze, A. et al., "Octane Appetite: The Relevance of a Lower Limit to the MON Specification in a Downsized, Highly Boosted DISI Engine," SAE Int. J. Fuels Lubr. 7(3):2014, doi:10.4271/2014-01-2718.
- [13] Kalghatgi, G., "Fuel/Engine Interactions," SAE International, Warrendale, PA, ISBN 978-0-7680-6458-2, 2013, doi:10.4271/R-409.
- [14] Kalghatgi, G., Head, R., Chang, J., Viollet, Y. et al., "An Alternative Method Based on Toluene/n-Heptane Surrogate Fuels for Rating the Anti-Knock Quality of Practical Gasolines," SAE Int. J. Fuels Lubr. 7(3):2014, doi:10.4271/2014-01-2609.
- [15] Chongming Wang, Soheil Zeraati-Rezaei, Liming Xiang, Hongming Xu, "Ethanol blends in spark ignition engines: RON, octane-added value, cooling effect, compression ratio, and potential engine efficiency gain," Applied Energy, Volume 191, 2017, Pages 603-619, ISSN 0306-2619, <https://doi.org/10.1016/j.apenergy.2017.01.081>.
- [16] Mittal, V. and Heywood, J., "The Relevance of Fuel RON and MON to Knock Onset in Modern SI Engines," SAE Technical Paper 2008-01-2414, 2008, <https://doi.org/10.4271/2008-01-2414>.
- [17] Mittal, V., Heywood, J., and Green, W., "The Underlying Physics and Chemistry behind Fuel Sensitivity," SAE Int. J. Fuels Lubr. 3(1):256-265, 2010, <https://doi.org/10.4271/2010-01-0617>.



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