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II. Co-Optimization of Fuels and Engines

II.1 Alternative Fuels DISI Engine Research: Autoignition Metrics

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Project Introduction

Improved engine efficiency is required to comply with future fuel economy standards. Alternative fuels have the potential to enable more efficient engines while addressing concerns about energy security. This project contributes to the science base needed by industry to develop highly efficient direct injection spark igniton (DISI) engines that also beneficially exploit the different properties of alternative fuels. Here, the emphasis is on quantifying autoignition behavior for a range of spark-ignited engine conditions, including directly injected boosted conditions. The efficiency of stoichiometrically operated spark ignition engines is often limited by fuel-oxidizer end-gas autoignition, which can result in engine knock. A fuel's knock resistance is assessed empirically by the Research Octane Number (RON) and Motor Octane Number (MON) tests. By clarifying how these two tests relate to the autoignition behavior of conventional and alternative fuel formulations, fuel design guidelines for enhanced engine efficiency can be developed.

Objectives

- Provide the science base needed by industry to understand how emerging alternative fuels impact autoignition in highly efficient DISI light-duty engines being developed by industry
- Develop and apply knock testing methodologies that are relevant for both transient and steady-state engine operation
- Measure knock limits for a range of fuels with varying octane rating and compositions
- Assess the applicability of the Octane Index framework to rank order fuels, including an assessment of measurement uncertainty

Approach

The Alternative Fuels DISI Engine Lab at Sandia houses an engine that is capable of both performance testing and in-cylinder optical diagnostics. Here, research is focused on performance testing with an all-metal fully lubricated engine configuration. The lab features in-house developed control and data acquisition hardware and software that are capable of complex engine operation, including load transients.

Results

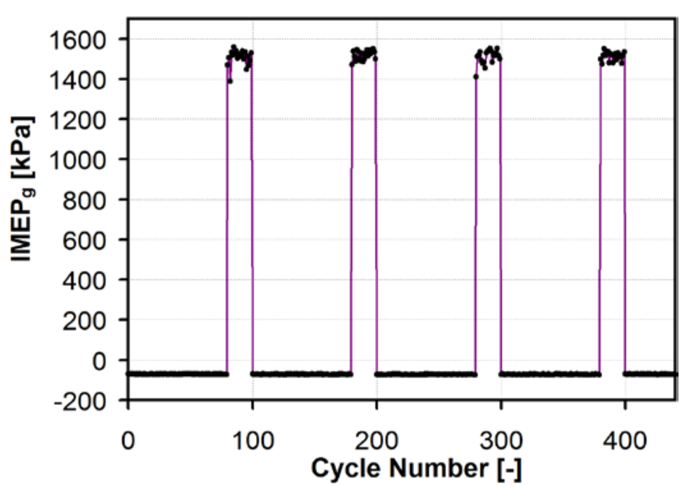
Key Accomplishments for Fiscal Year 2017

- Developed methodology to measure knock limits under conditions that mimic vehicle accelerations
- Measured stoichiometric knock limits for nine fuels, both steady-state and transient
- Tested applicability of Octane Index framework for fuels of alternate composition and discovered that two fuels blended with butanol isomers performed better than expected based on RON and MON
- Developed and used a Monte-Carlo-based uncertainty assessment of the Octane Index framework; results indicate a high likelihood that fuels' deviations from Octane Index predictions are real and not caused by experimental uncertainty

In the following sections, detailed examples of Fiscal Year 2017 accomplishments are presented.

Knock-Limited Stoichiometric Operation

The knock limits of stoichiometric charge DISI engines have a significant effect on engine efficiency. Fuels exhibit varying degrees of knock resistance depending on their composition and this is quantified by RON and MON ratings. However, while knock-limited testing is nearly exclusively performed under steady-state conditions, real engines experience transient conditions, especially those found in light-duty vehicles. This mismatch could affect the real-world performance of fuels due to the difference in conditions between transient high-load operation and steady-state high load operation, with the key difference being the higher thermal state of the engine under steady-state conditions. To investigate the differences between transient and steady-state operation, a transient test regime was developed and experiments were performed over a range of steady-state and transient conditions. The particular transient test regime implemented here was chosen to magnify differences between steady-state and transient operation by producing a marked shift in engine thermal state. This is accomplished by firing 20 cycles under knock-limited conditions, followed by 80 cycles of motoring, in which no fuel is injected and no combustion occurs, as illustrated in Figure II.1.1. This 20% duty cycle of the engine results in lower in-cylinder wall temperatures and higher volumetric efficiency, which reflect the lower thermal state of the engine (Vuilleumier and Sjöberg 2017). A secondary benefit of this transient test regime is the ability to test higher load conditions than are possible to test under steady-state conditions, due to the reduced knocking tendency at lower thermal conditions.



$IMEP_G$ – gross indicated mean effective pressure

Figure II.1.1 - Illustration of repeating Fire20-Skip80 sequence used to mimic the thermal state that an engine may experience during vehicle acceleration. Figure by Magnus Sjöberg.

Measured knock-limited combustion phasing (KL-CA50) from both steady-state and transient testing at a fixed engine speed (1,400 rpm) and intake temperature (30°C) are presented in Figure II.1.2. KL-CA50 indicates the combustion phasing which causes a predetermined knocking threshold to be met; lower KL-CA50 values indicate that a fuel is less knock limited. Figure II.1.2 presents data taken with nine fuels, which have their properties listed in Table II.1.1. Of the fuels, eight fuels share a RON rating of 98 and seven of these fuels share octane sensitivity (S) ratings, the difference of RON and MON ratings, of approximately 10. The ninth fuel included in this test matrix is an E10 (10% ethanol, 90% gasoline) blend mimicking regular grade pump gasoline.

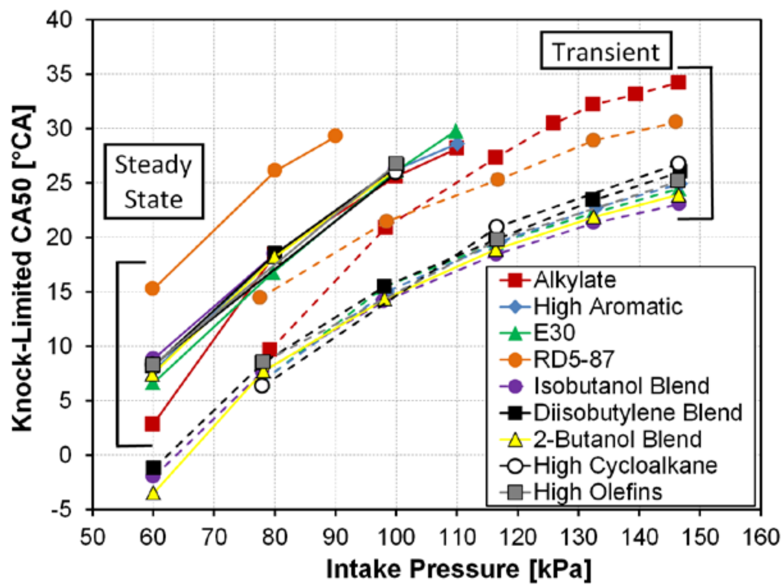


Figure II.1.2 - Knock-limited combustion phasing as a function of intake pressure for both steady-state and transient operation with 30°C intake temperature. Transient operation is shown in dashed lines. Figure by David Vuilleumier, SNL.

Figure II.1.2 shows that under steady-state, naturally aspirated conditions, the RON = 98 fuels perform nearly identically to one another. However, as conditions shift to throttled operation, or to transient conditions, divergence in fuel performance is observed. Of particular interest is the spread in behavior of the RON = 98, S = 10 fuels at the highest tested intake pressure, which raises questions about the use of RON and MON to describe fuel knock resistance. Of further interest is the crossover in relative knock performance between the alkylate fuel (RON = 98, S = 1) and the RD5-87 (RON = 92, S = 7), which indicates that knock resistance must be described in relation to the conditions encountered by the fuel.

While Figure II.1.2 shows the knock limits of the nine fuels, Figure II.1.3 plots the corresponding indicated efficiencies. The measured efficiencies are a function of many factors, including throttling losses, thermodynamics, average charge temperature, and combustion efficiency. However, under knock-limited conditions, which can force the use of non-optimal combustion phasing, the knock resistance of a fuel has an outsize effect on its efficiency. This is reflected in Figure II.1.3, which shows that under steady-state conditions, where the RON = 98 fuels behaved similarly to one another, similar efficiencies are observed. Conversely, with transient operation, where differences in knock-resistance were noted, indicated efficiency also varies among the fuels with the most knock resistant fuels having relative efficiency gains of approximately 10% over the regular grade gasoline.

Octane Index Applicability

As previously noted, the crossover in performance of the alkylate and RD5-87 as intake pressure changes, shown in Figure II.1.2, indicates that a single rating of a fuel is insufficient to describe its behavior. The leading methodology for describing fuel anti-knock quality with regards to conditions is the Octane Index (Kalghatgi 2001), which is presented in Equation 1. This approach considers both the RON and MON rating of a fuel, as well as a weighting factor, K, which is dependent on the conditions the fuel is subject to. It may be

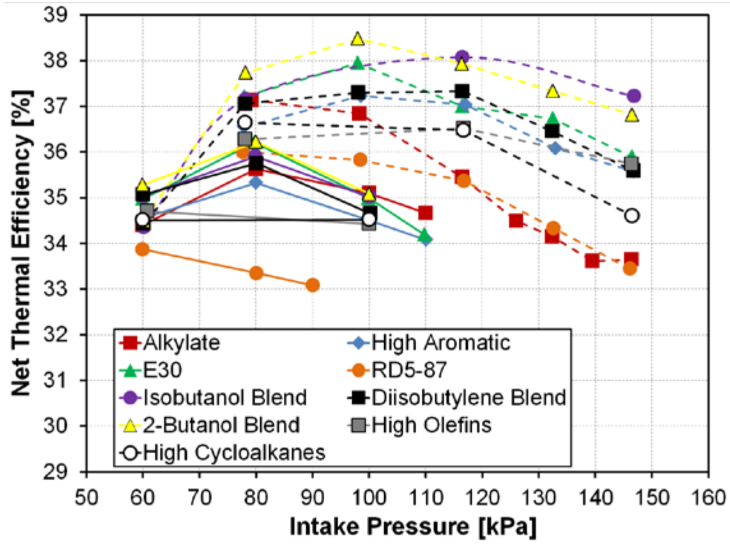


Figure II.1.3 - Indicated thermal efficiency as a function of intake pressure for all nine fuels for both steady-state and transient operation. Transient operation is shown in dashed lines. Figure by David Vuilleumier, SNL.

observed that when K = 1, the Octane Index value is the same as the MON rating, while if K = 0, the Octane Index value is equal to the RON rating.

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

The K term in the Octane Index equation is an empirical term, although it is generally related to the conditions experienced by the end gas with higher temperatures and lower pressures raising the K value and vice versa. Nonetheless, K must be calculated by a regression (typically linear) between a parameter which indicates the knock resistance of a fuel (such as the knock-limited combustion phasing, knock-limited spark advance, knock-limited vehicle acceleration, etc.) and the Octane Index value of a fuel. However, each of the parameters which feed into the regression has some uncertainty associated with it, such as a fuel's RON and MON ratings, or the knock metric. This uncertainty results in two questions: (1) how certain is the K value which is determined and (2) when discrepancies between the Octane Index and observed performance occur, is this a failing of the Octane Index methodology or is it caused by experimental uncertainty?

To answer these questions, the experimental data presented in the previous section were combined with Monte Carlo simulations to quantify the uncertainty associated with the Octane Index. The experimental results were used to perform a linear regression at each operating condition to determine the most appropriate K value. The Monte Carlo simulations piggybacked on the linear regression methodology by rerunning the linear regression at each operating condition for 100,000 permutations of the RON, MON, and KL-CA50 inputs, which are reflective of the uncertainty in each of these terms.

An example of the linear regression between Octane Index and KL-CA50 is shown in Figure II.1.4. This figure uses experimental data from the highest tested intake pressure of 146 kPa and plots the best-fit relationship between Octane Index and KL-CA50, which stems from K = -2.1, and results in an R^2 value of 0.84. This figure illustrates that while the Octane Index generally describes experimental results, some discrepancies exist and these may be due to the effects of fuel composition. Figure II.1.5 presents the distribution of R^2 values from the Monte Carlo simulations which are associated with the results shown in Figure II.1.4. Figure II.1.5 indicates that when the uncertainty of the measured parameters are considered, the linear regressions between KL-CA50 and Octane Index produce a range of R^2 values from approximately 0.7 to 0.9. Figure II.1.5 also indicates that it is extremely unlikely that the Octane Index would provide a perfect fit for the measured knock behavior, even when uncertainty is considered.

Figure II.1.6 summarizes the K-value uncertainty quantification results from the range of tested operating conditions. It may be seen from this figure how different experimental conditions influence K. Broadly, higher

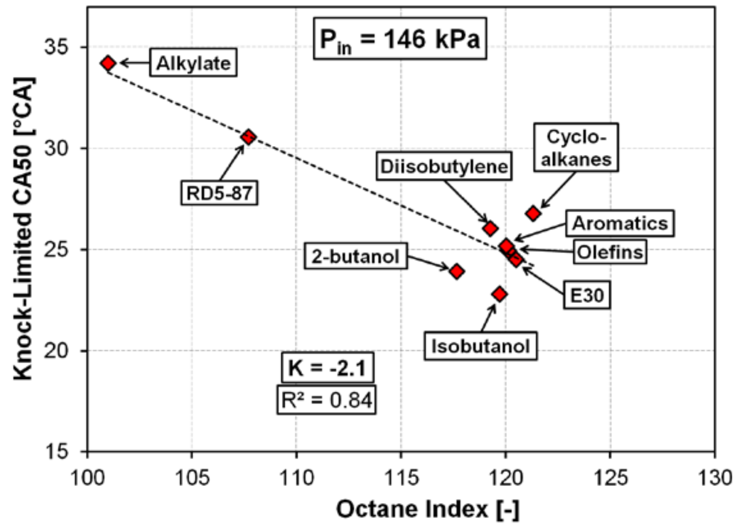


Figure II.1.4 - Best-fit linear regression between octane index and knock-limited combustion phasing for an intake pressure of 146 kPa under transient operation. Figure by David Vuilleumier, SNL.

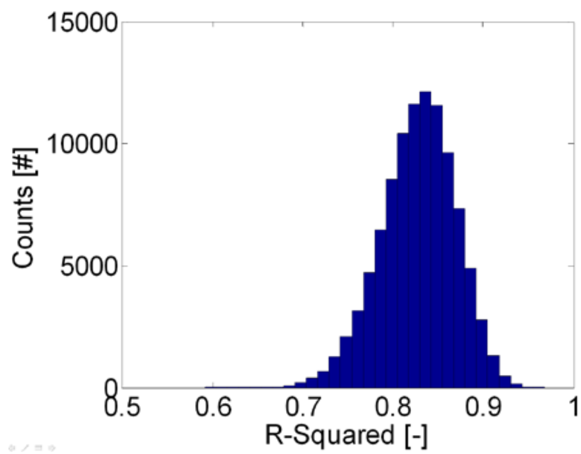


Figure II.1.5 - Distribution of R^2 values at the 146 kPa intake pressure, 30°C intake temperature, transient operating mode condition. Figure by David Vuilleumier, SNL.

intake pressure conditions reduce K as expected. Further, lower initial temperatures, such as those encountered in the transient operation, further reduce K. Figure II.1.6 shows that K becomes significantly negative for transient, boosted operating conditions. This has a major implication for fuel formulation. As turbocharged engines gain market share, they become knock-limited at conditions which are represented by negative values of K. At these conditions, fuels with a large difference between RON and MON ratings perform better than fuels which have a higher MON rating. This is not reflected in the way fuels are sold in the United States, as fuels are marketed by the average of RON and MON, which penalizes fuels with lower MON ratings for a given RON rating.

Finally, Figure II.1.6 also presents the 80% certainty range in the K-value. It can be seen that when the K-value ranges between 0 and 1, the uncertainty range spans approximately 0.2 units of K. However, as the K-value becomes negative and therefore relies on the extrapolation of RON and MON results, the uncertainty in K increases dramatically, such that at the most extreme condition tested, the 80% certainty range spans over two units of K. This presents a problem when determining the relative merits of two fuels for a downsized-boosted engine; depending on the magnitude of K, a higher-RON lower-S fuel may perform better, or a lower-RON higher-S fuel may perform better.

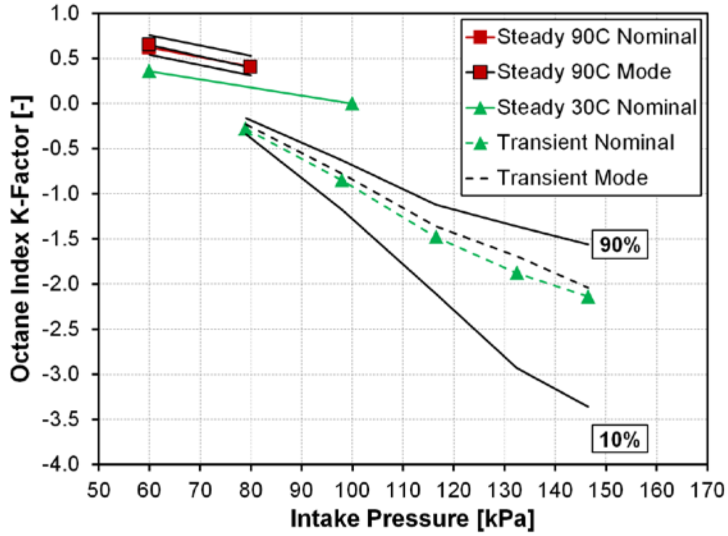


Figure II.1.6 - K-values as a function of intake pressure and operation type accompanied by the 10th and 90th percentiles of the K distribution, as well as the mode of the distribution. Figure by David Vuilleumier, SNL.

Table II.1.1 - Fuel Properties and Composition for the Nine Fuels Used in This Study

	Iso-butanol blend	2-butanol blend	Diisobutylene blend	Alkylate	E30	High Aromatic	High Olefins	High Cyclo-alkanes	RD5-87
RON	98.1	98.2	98.3	98.0	97.9	98.1	98.3	97.8	92.1
MON	88.0	89.1	88.5	96.7	87.1	87.6	87.9	86.9	84.8
AKI (R+M)/2	93.1	93.7	93.4	97.3	92.5	92.8	93.1	92.3	88.5
Octane Sensitivity	10.1	9.1	9.8	1.3	10.8	10.5	10.4	11.0	7.3
Aromatics (Vol. %)	19.0	17.9	20.1	0.7	13.8	39.8	13.4	33.2	21.5
Olefins (Vol. %)	3.8	3.6	23.6	0.1	5.6	4.5	26.5	1.6	5.7
Alkanes (Vol. %)	53.1	50.1	56.3	98.8	40.5	46.2	56.4	40.6	49.0
Cycloalkanes (Vol. %)	0	0	0	0	7.0	8.0	2.9	24.2	11.4
Oxygenates (Vol. %)	24.1	28.4	0	0	30.4	0	0	0	10.2
Heat of Vaporization (kJ/kg)	412*	415*	337*	308*	532*	361*	333*	373*	-

*Heat of vaporization data provided by Fioroni et al.

Conclusions

This project used both existing and newly developed methodologies to assess the knock resistance of nine fuels over a wide range of engine operating conditions. Beyond the experimental data provided here, uncertainty quantification was carried out to assess the performance of a leading fuel classification scheme, the Octane Index, in describing the observed behavior. The following findings are noted:

- A transient test methodology was developed for autoignition studies which simulates a brief but sometimes aggressive load transient.
- Transient operation allows the investigation of high-load, boosted, beyond RON conditions while using a relatively high compression ratio of 12.
- Differences in fuel knock resistance are observed under high-load conditions which uncertainty analysis confirmed are not explained by the RON and MON ratings of the fuels.
- In the Octane Index framework, extrapolation of RON and MON results leads to high uncertainty in computed K values, undermining the ability of the Octane Index to rank order fuel performance at these extreme conditions.

- The two fuels blended with iso-butanol and 2-butanol overperform their RON and MON ratings at boosted engine-operating conditions.

References

Fioroni, G., L. Fouts, E. Christensen, R. McCormick, NREL, Private Communication, February 16, 2017.

Kalghatgi, G. “Fuel Anti-Knock Quality - Part I. Engine Studies.” SAE Technical Paper 2001-01-3584, 2001, doi: 10.4271/2001-01-3584.

Vuilleumier, D. and M. Sjöberg. “The Use of Transient Operation to Evaluate Fuel Effects on Knock Limits Well Beyond RON Conditions in Spark-Ignition Engines.” SAE paper 2017-01-2234.

Key Fiscal Year 2017 Publications

116. Vuilleumier, D. and M. Sjöberg. “Significance of RON, MON, and LTHR for Knock Limits of Compositionally Dissimilar Gasoline Fuels in a DISI Engine.” *SAE Int. J. Engines* 10(3), 2017.

117. Sjöberg, M., and Xu He. “Combined Effects of Intake Flow and Spark-Plug Location on Flame Development, Combustion Stability and End-gas Autoignition for Lean SI Engine Operation using E30 Fuel.” ENCOM 2017.

118. Vuilleumier, D. and M. Sjöberg. “The Use of Transient Operation to Evaluate Fuel Effects on Knock Limits Well Beyond RON Conditions in Spark-Ignition Engines.” SAE paper 2017-01-2234.

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