

Fuel/Engine Interactions: Potential for Emissions and Efficiency Benefits Part1: SI Fuels

Paul Miles

Combustion Research Facility
Sandia National Laboratories

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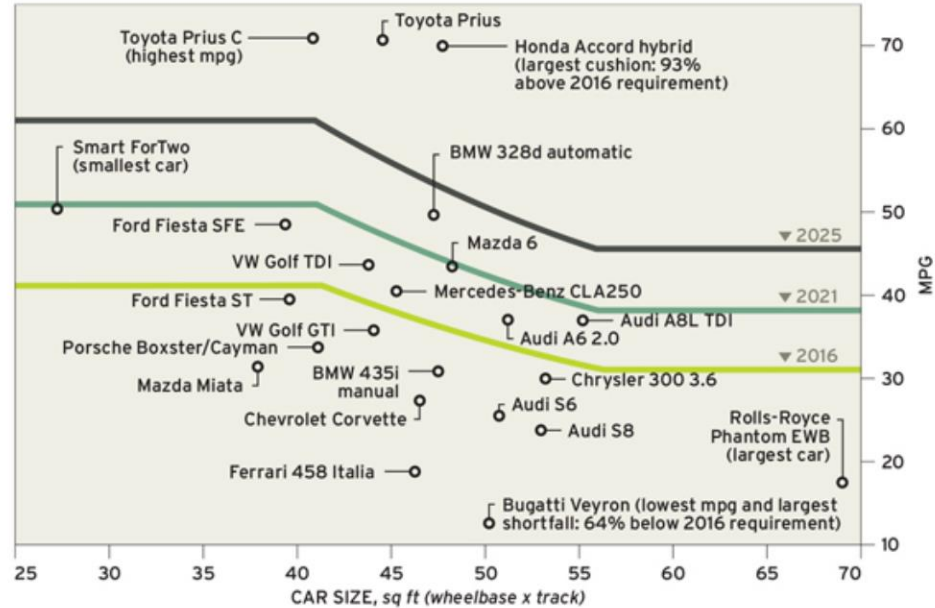
Acknowledgments:

- Gurpreet Singh, Kevin Stork, Leo Breton – Program Managers, DOE EERE Vehicle Technologies Office
- USCAR Advanced Combustion and Emission Control Tech Team Subcommittee on Fuel Effects*

* The views represented here do not represent official views of USCAR or the ACEC Tech Team

Motivation

- 2025 vehicles must halve their fuel consumption compared to 2010 vehicles
 - **Improved** fuels offer potential to design engines for greater efficiency
 - **Renewable** fuels offer additional advantages related to sustainability and climate change



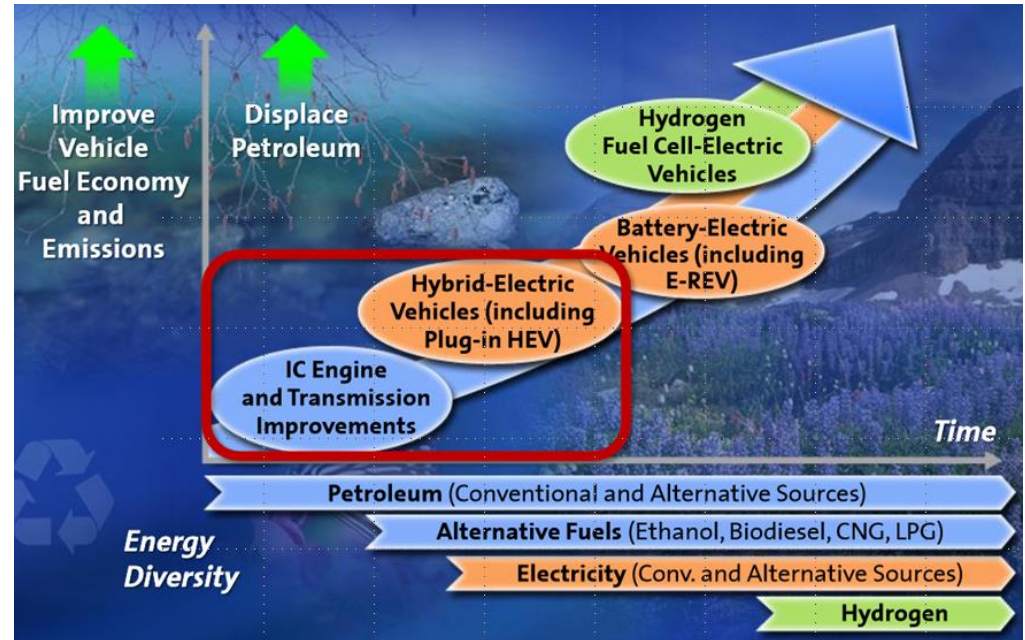
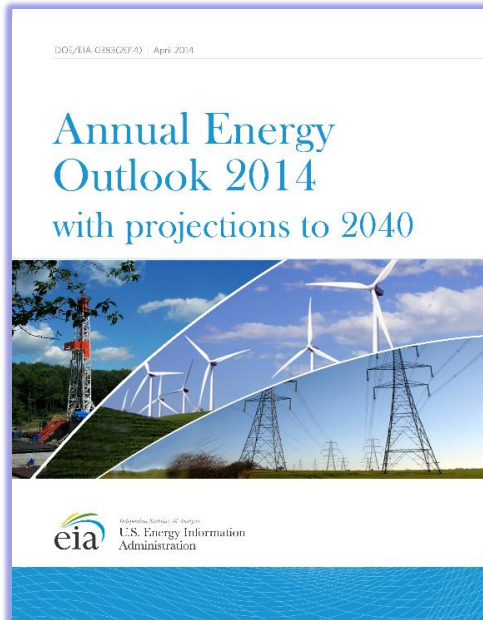
Source: <http://blog.caranddriver.com>

Questions:

- What kind of engine efficiency gains are possible?
- What fuel properties are needed to enable these gains?
- What additional research is needed to permit engine-fuel co-optimization?

What do we believe the vehicle fleet will look like in 2025?

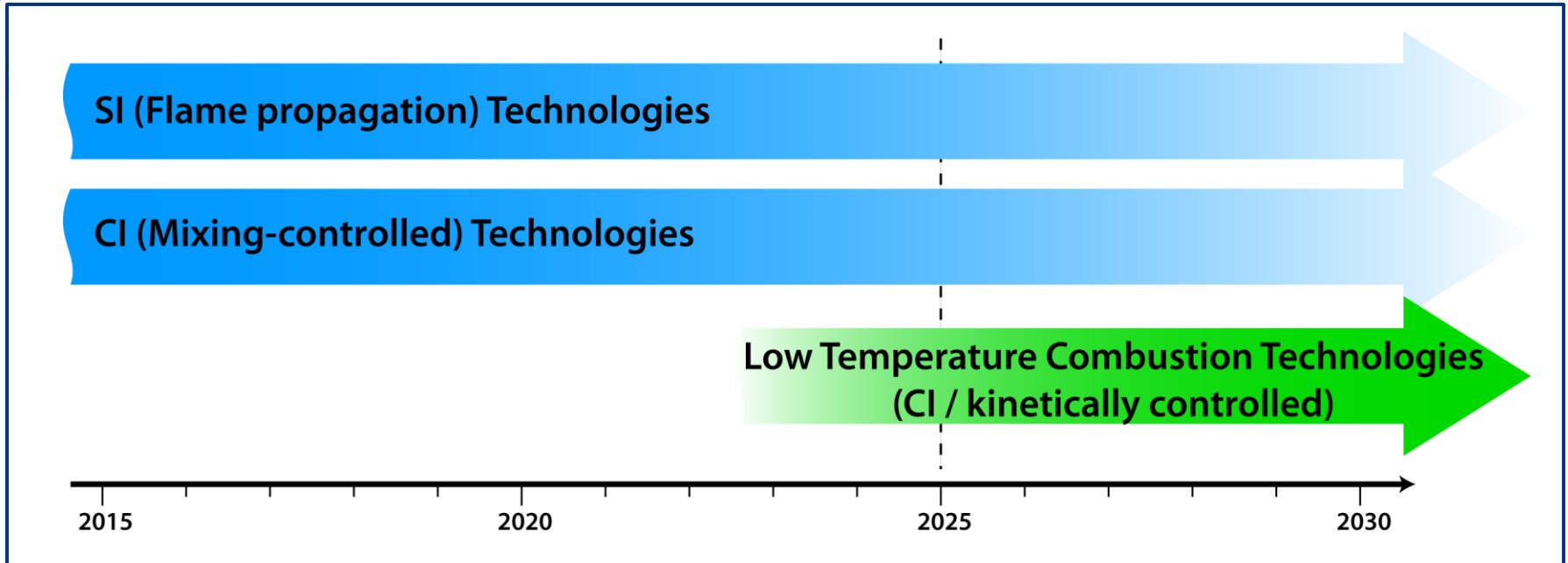
Both industry and government anticipate that IC engines continue to be a significant fraction of the fleet



GM (Gary Smythe, UW Symp. 2011)

EIA AEO 2014 reference case scenario: even by 2040, **over 99% of vehicles sold will have ICEs**

We expect multiple IC engine technologies to co-exist in the marketplace



- Each engine technology may be optimized for various applications:
 - Downsized, boosted for maximum fuel efficiency
 - Naturally aspirated for low-cost markets
 - Hybrid applications
- Paths might merge as technologies mature (e.g. SACI; late-injection LTC, GCI)



Impact of fuel properties on SI engine technologies will be dominated by Octane

The effect of increasing fuel octane number on engine and vehicle energy efficiency cannot be quantified in a simple way but requires a complex, nuanced answer

K. G. DULEEP

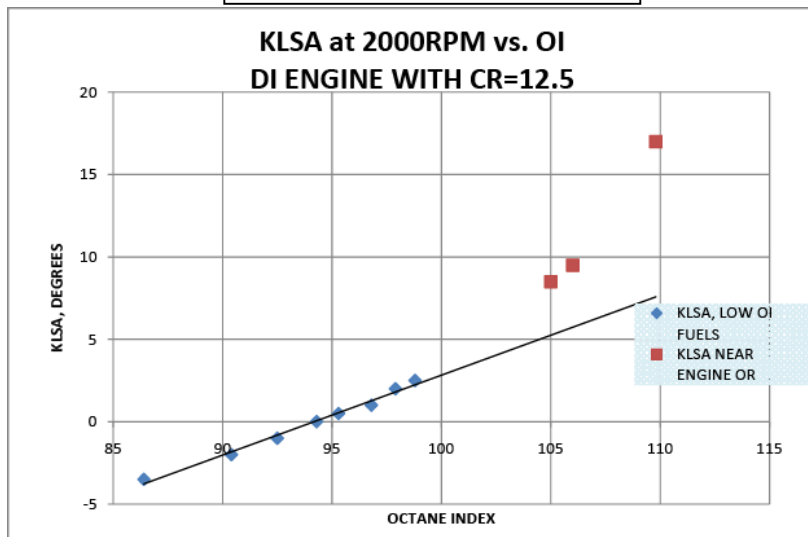
CRC Final Report

Project CM-137-11-1b, 2012

Resistance to autoignition is one key to efficiency improvement in SI engines

$$\eta_{th} = 1 - \frac{1}{r_c^{\gamma-1}} \left[\frac{\alpha \beta^{\gamma} - 1}{\alpha \gamma (\beta - 1) + \alpha - 1} \right]$$

CRC CM-137-11-1b 2012



- Higher octane number allows higher compression ratio r_c (improved efficiency when engine is not knock-limited)
- Higher octane also allows greater knock-limited spark advance at fixed r_c (improved efficiency at high-load)

Choice of r_c depends on duty-cycle, boost, bore, mixing, heat transfer, exhaust pressure, chamber geometry...

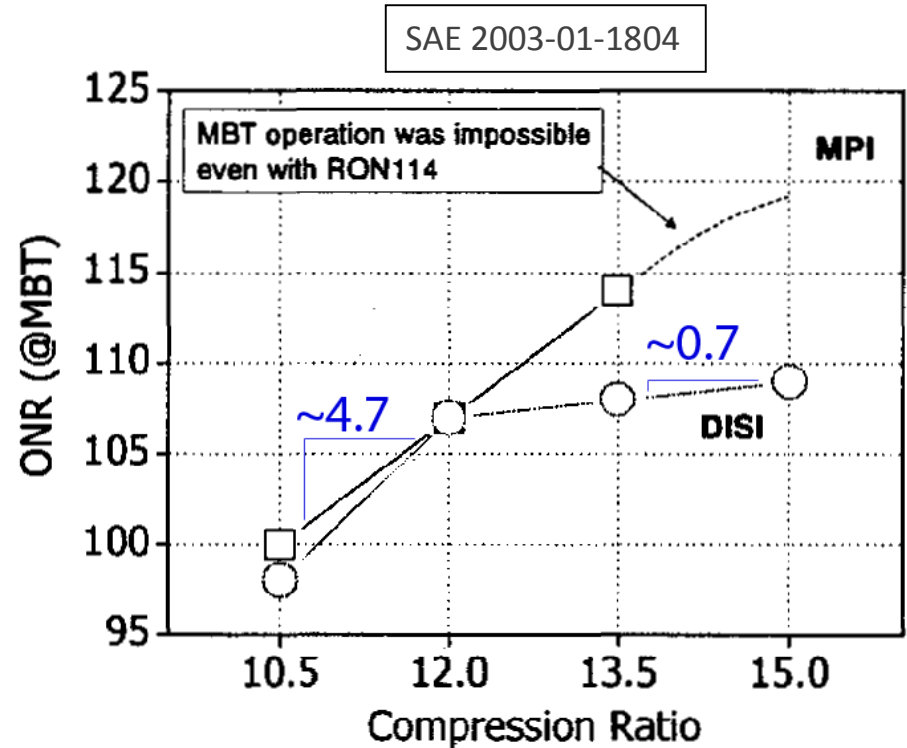
What increase in ON is needed to increase r_c ?

- Estimates in the literature vary widely, and depend on engine technology, geometry, & operating condition
- Prior surveys indicate 4-5 RON is needed per point of r_c

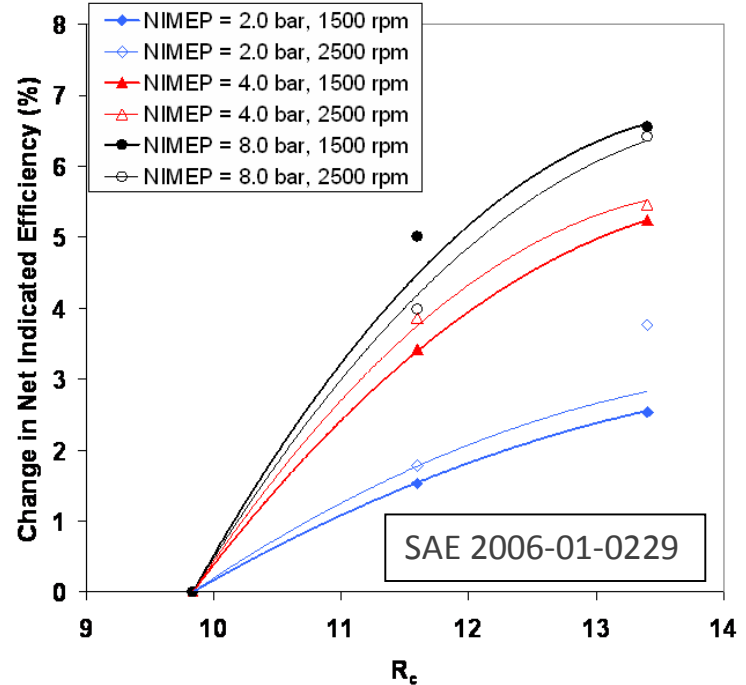
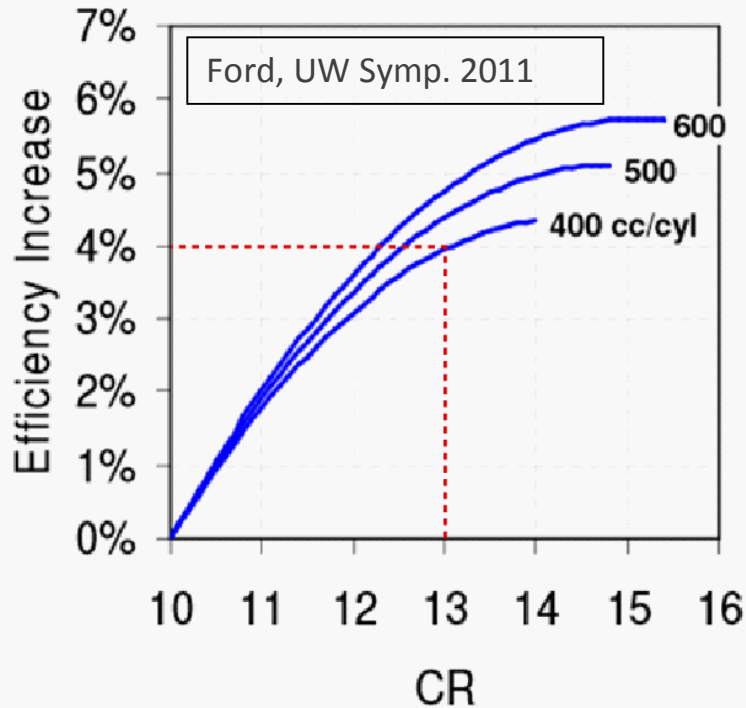
SAE 2014-01-1961
CRC CM-137-11-1b

- A recent review suggests $\sim 3 \text{ ON}/r_c$
 - Controlled studies with modern PFI & DI engine technology
 - Consistent design practices as r_c is varied

Leone, et al. , submitted



How much efficiency can be gained per unit increase in r_c at fixed displacement?



- Efficiency gain depends on displacement, speed & load...
- Diminishing returns as CR increase (increasing surface-volume ratio)
- ~2% increase in relative efficiency per unit r_c seems a consensus value. Will use **1.6%** as a more conservative estimate
- Independent of method of fuel induction (PFI or DI)



Higher octane also enables higher boost at fixed r_c , facilitating downsizing

Engine downsizing allows the engine to run at more efficient, higher load operating points

- The Douad-Eyzat auto-ignition integral shows that, for gasoline-like fuels:

$$P_2 = P_1 \left(\frac{RON_2}{RON_1} \right)^2$$

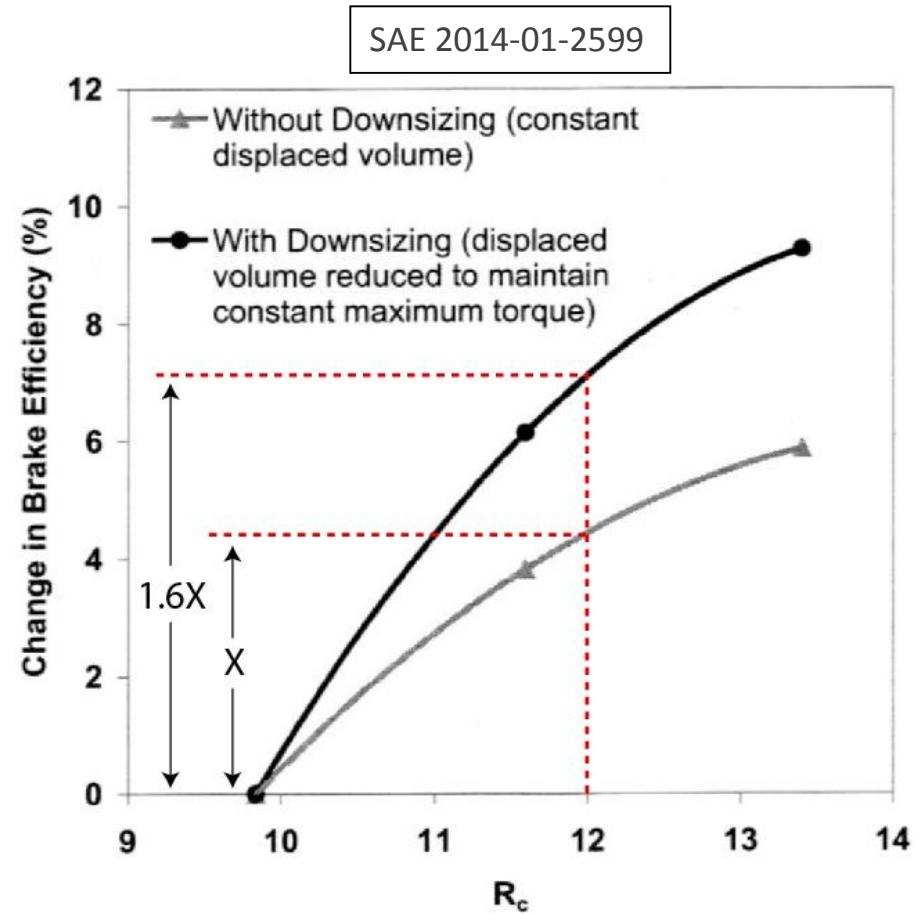
$$\tau = A * \left(\frac{RON}{100} \right)^{3.4} P^{-1.7} \exp\left(\frac{3800}{T} \right)$$

- Increasing RON from 91 to 100 allows a 21% increase in pressure at a fixed autoignition time

Increased efficiency also enables downsizing at constant boost

- If the engine remains equally knock-limited, for equal airflow the torque increases due to the efficiency increase
- Increased torque allows engine downsizing *or* downspeeding
- The **efficiency multiplier** due to downsizing varies in the literature
- A recent review paper suggests:
 - 1.3X (naturally aspirated)
 - 1.1X (turbocharged)

Leone, et al., submitted





So far, we have been talking about RON – Where does MON fit in?

Background

- Research and Motor Octane Numbers (RON and MON) are measured according to ASTM D2699 and D2700
- Both tests compare the test fuel to a blend of *iso*-C₈H₁₈ and *n*-C₇H₁₆; the RON or MON is the percentage of *iso*-C₈H₁₈ that provides the same knock characteristics
- The pump octane number or anti-knock index is (RON+MON)/2
- The most essential difference between the RON and MON tests is the intake temperature and where it is regulated:
RON: $T_{in}=52^{\circ}\text{C}$, upstream of carburetor
MON: $T_{in}=149^{\circ}\text{C}$, downstream of carburetor

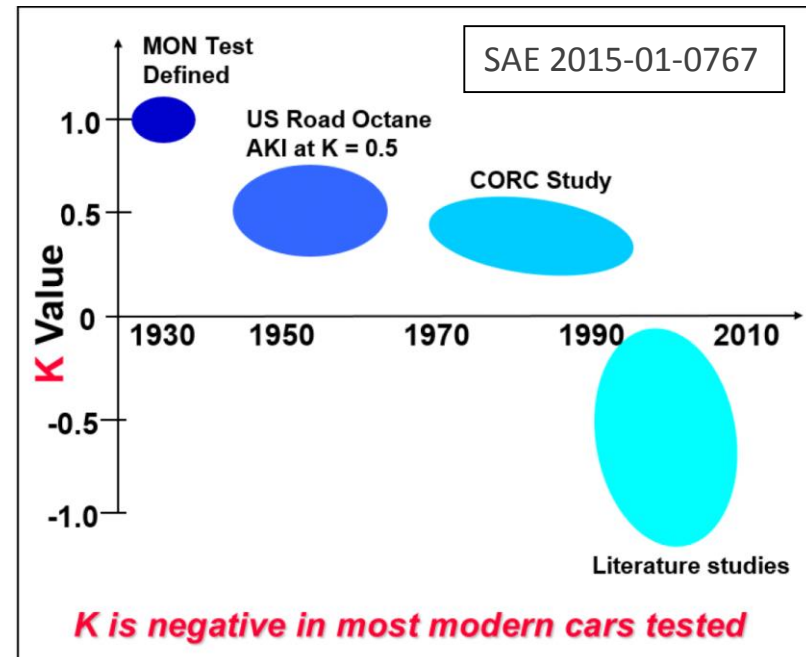


The Octane Index (OI) and fuel sensitivity

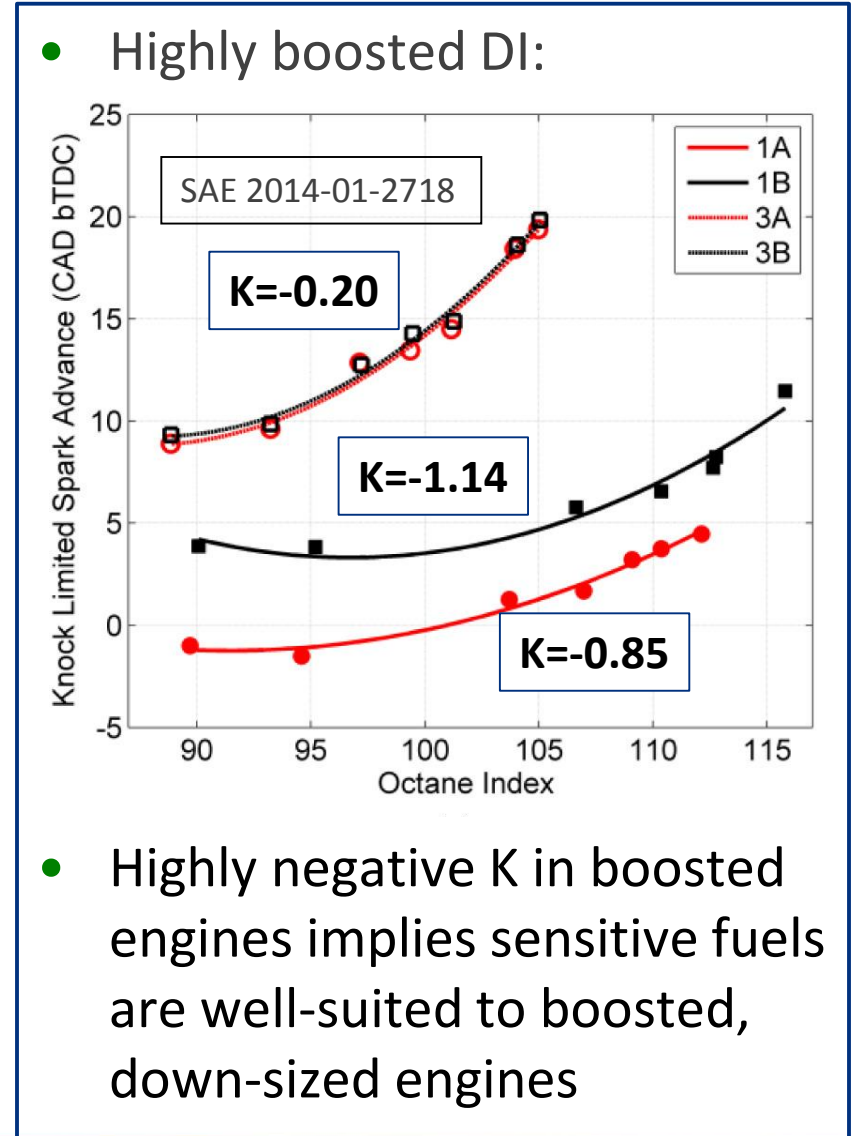
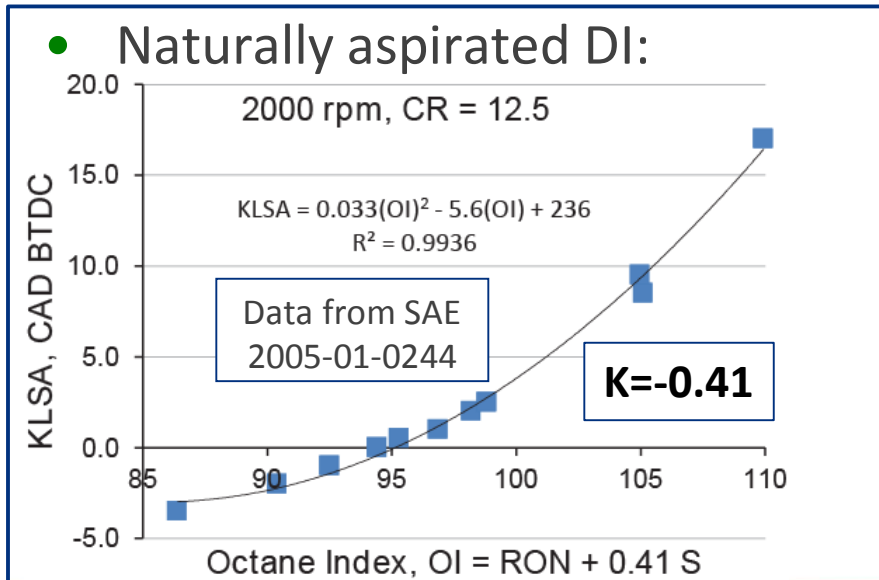
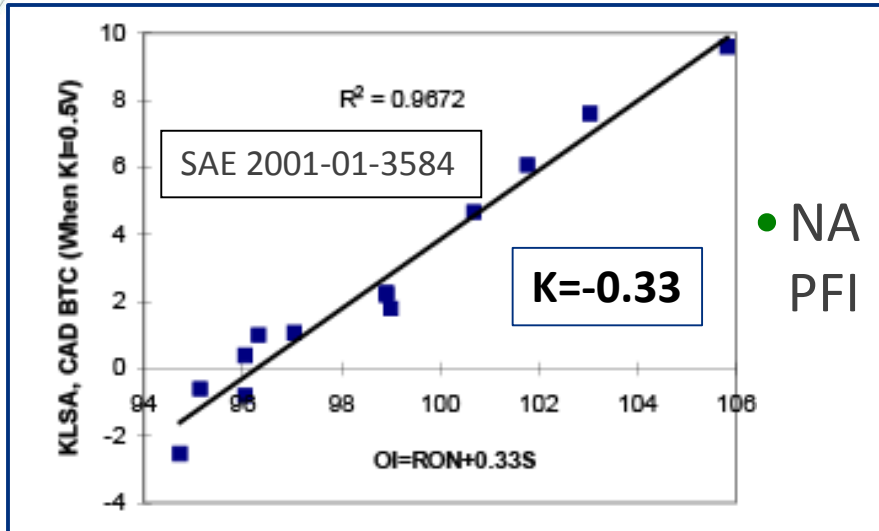
- OI is considered a measure of the true antiknock quality of a gasoline

$$OI = (1-K) * RON + K * MON = RON - K * (RON - MON)$$

- K is an empirical *engine* constant, which depends “*only*” on the P & T history of the unburned mixture (speed, engine, boost, T_{intake} , etc.)
- When $K=0$, the P & T history is RON-like and $OI = RON$
- When $K = 1$, the P & T history is MON-like and $OI = MON$
- K essentially *interpolates* the octane rating for conditions between the RON and MON test: if $K>1$ or $K<0$ we are *extrapolating*
- Does OI continue to represent the fuel anti-knock quality?



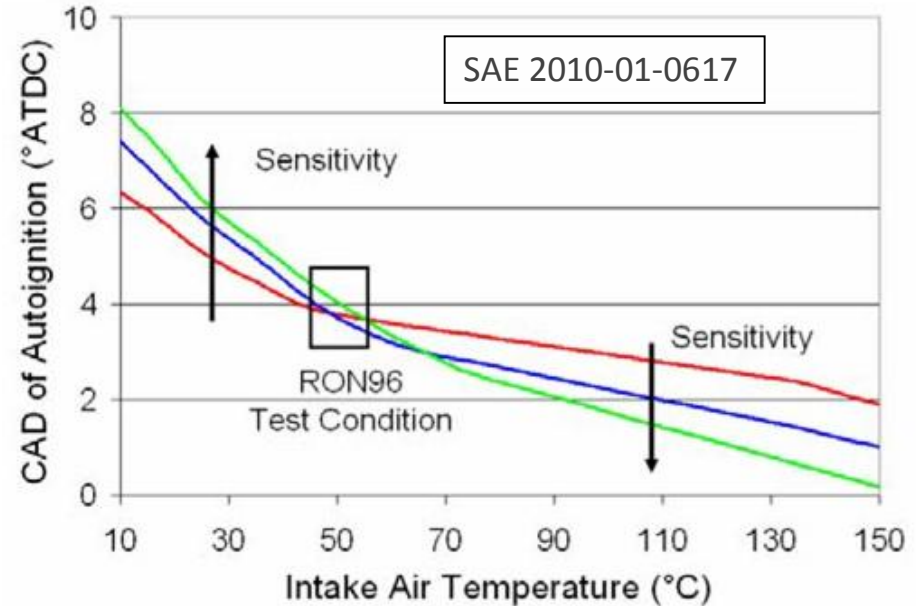
Yes. Correlations of KLSA with OI are much better than with RON alone



- Highly negative K in boosted engines implies sensitive fuels are well-suited to boosted, down-sized engines

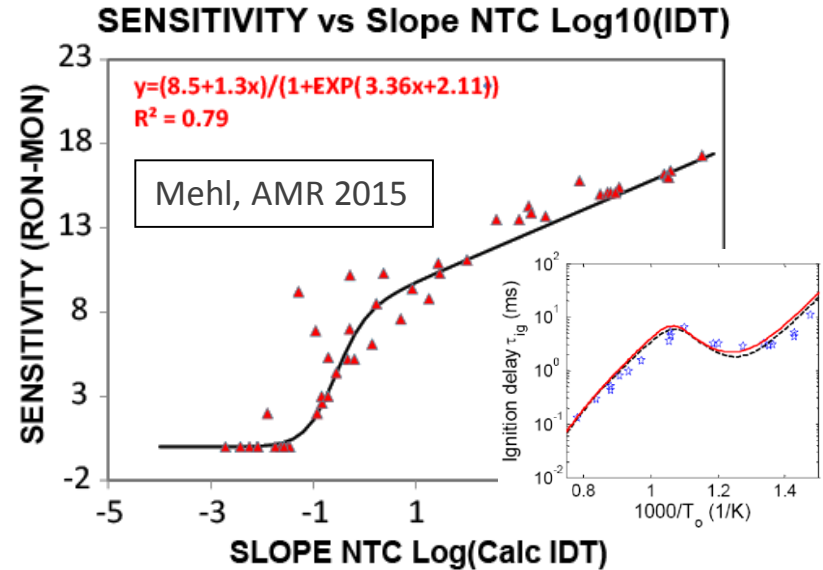
K multiplies the fuel “sensitivity”, RON-MON, in determining the OI

- “Sensitivity” is the sensitivity of the fuel to the end-gas temperature/pressure history
- Less sensitive fuels show a lower sensitivity of the auto-ignition delay due to temperature
- At conditions cooler than the RON test ($K < 0$), sensitive fuels (low MON) show better auto-ignition resistance
- At conditions hotter than the RON test ($K > 0$), less sensitive fuels (high MON) show better auto-ignition resistance
- K can be positive or negative in the same engine, depending on operating conditions (not clear that very low/high MON is always good)



Sensitivity appears related to the temperature and pressure dependencies of the ignition delay

- Fuel sensitivity correlates with the slope of ignition delay ν temperature in the NTC region
- For highly sensitivity fuels a larger change in ignition delay occurs for a unit change in sensitivity
- Pressure also influences auto-ignition, and there is some evidence that sensitive fuels have a low pressure exponent



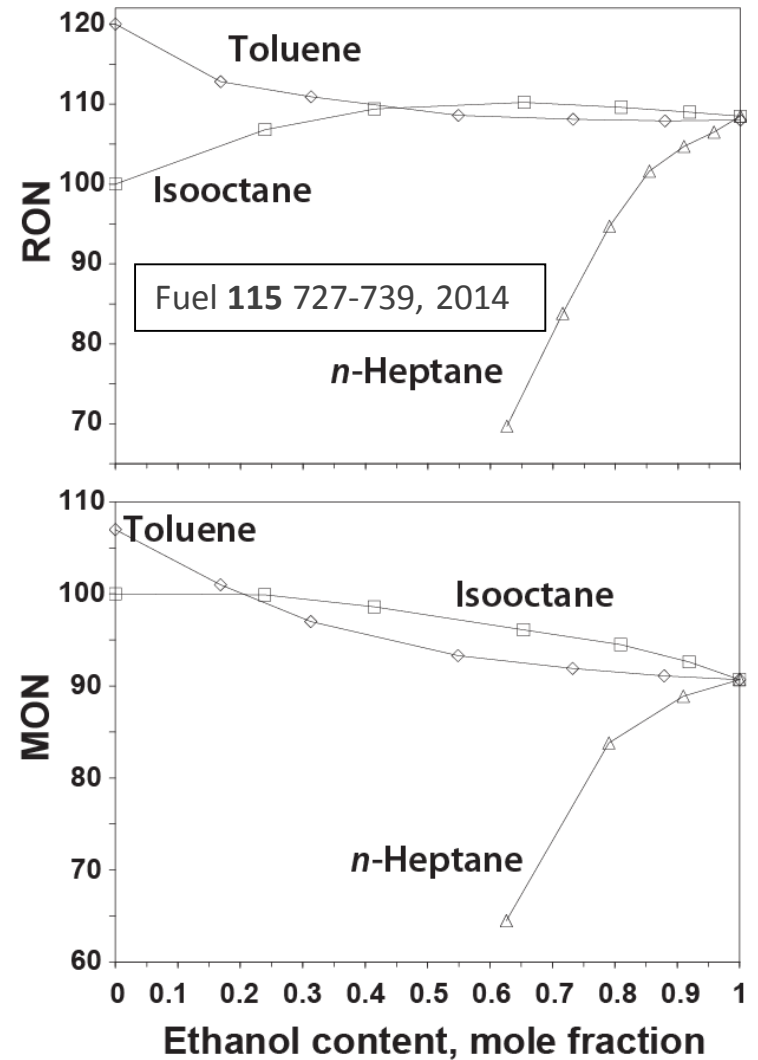
$$\tau = A * RON^B P^{-x} \exp\left(\frac{3800}{T}\right)$$

Fuel	x
Gasoline	1.7
1-hexene	~0.40

A better understanding of the origins of fuel sensitivity is needed before we can predict fuel behavior in an engine

Blending can also have unanticipated effects on octane number

- Synergistic (with PRFs) and antagonistic (with toluene) blending effects of ethanol and other alcohols
 - Can potentially explain discrepancies in the literature regarding non-linearity in RON with ethanol mole fraction
- Need understanding of the kinetic interactions in the LTHR and ITHR regions that impact auto-ignition





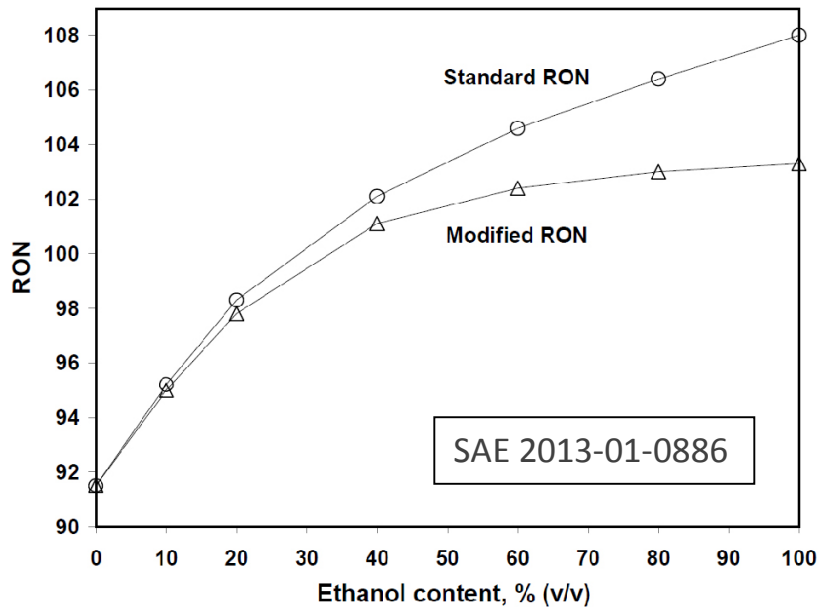
Wrapping up OI, K, & sensitivity...

- Despite large differences in the detailed chemical composition of the fuel, the OI formulation is a useful predictor of fuel behavior
- The OI is difficult to relate to the fundamental auto-ignition properties of the fuel
- Any improved auto-ignition metric will need to closely correlate with RON and MON to be readily accepted
- Some evidence that low MON (high-sensitivity) fuels are more susceptible to hot-spot pre-ignition
- Increasing MON is an energy intensive process, so high sensitivity fuels may have additional well-to-wheel efficiency advantages

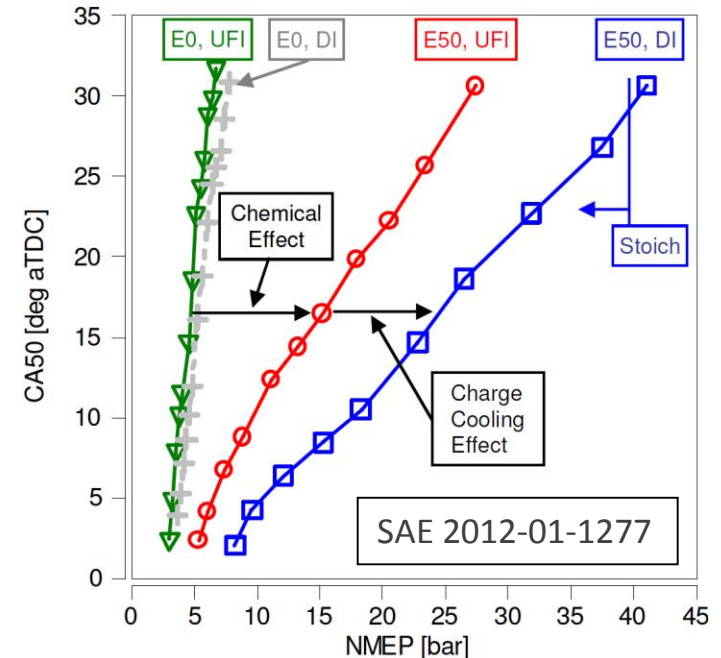
An increase in sensitivity from 8 to 14, say, coupled with a modern engine with $K \sim -0.5$, is equivalent to a **RON increase of 3**

Phase change properties: heat of vaporization (HoV)

- The literature is ambiguous regarding the impact of HoV on knock resistance
(Ethanol has $\sim 4.5X$ the HoV of gasoline per unit mass stoich. charge)



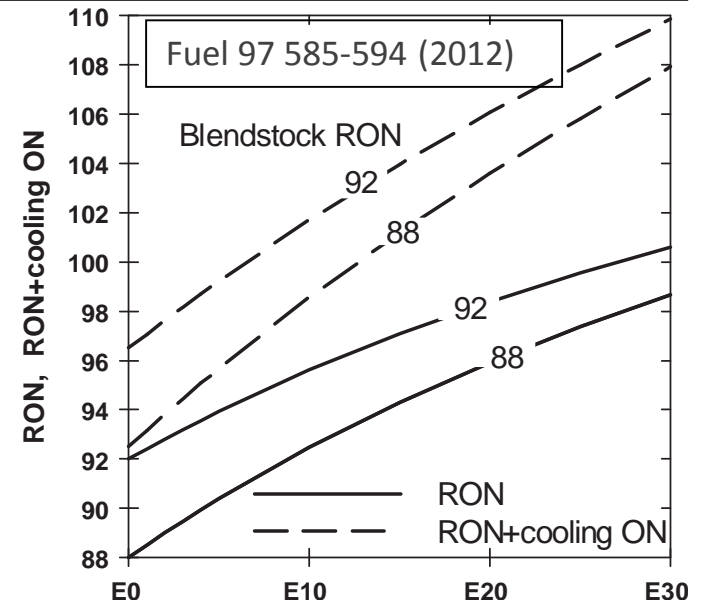
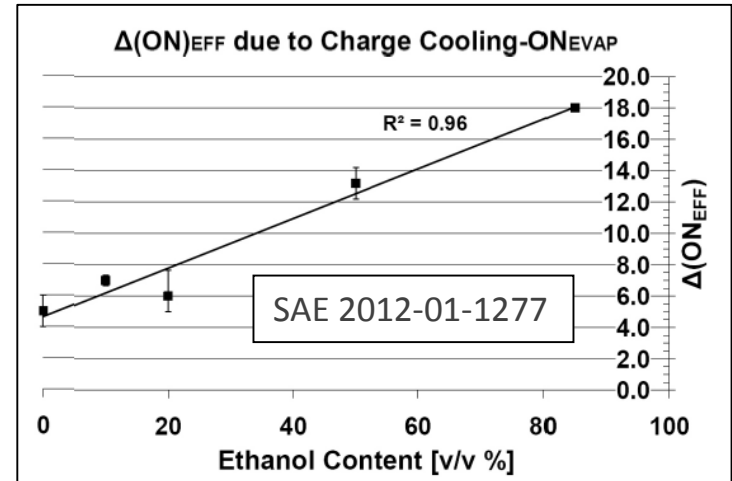
- A modified RON test regulating the mixture temperature shows a Δ RON of only ~ 2 for E50



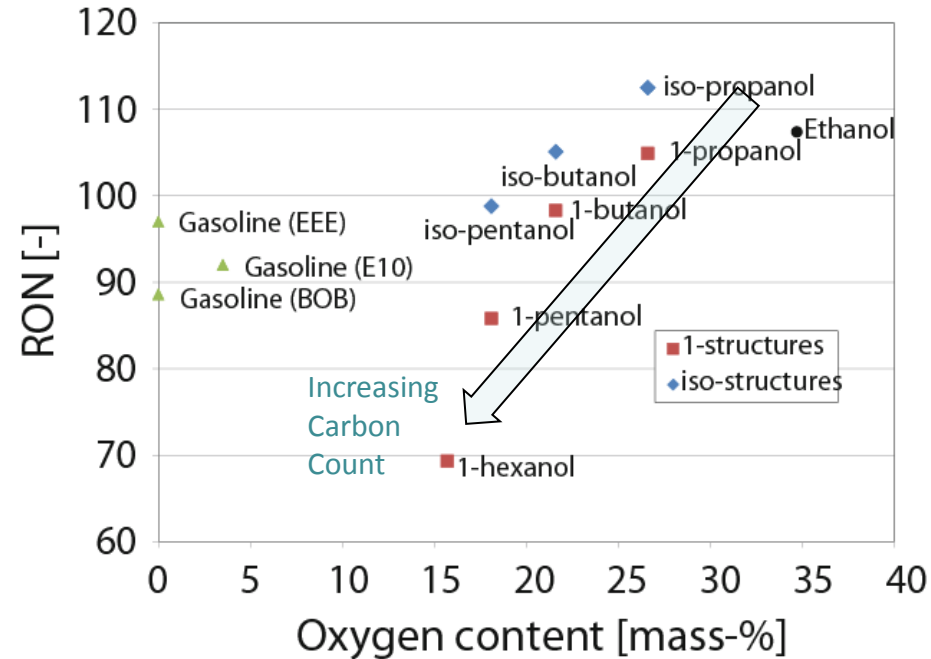
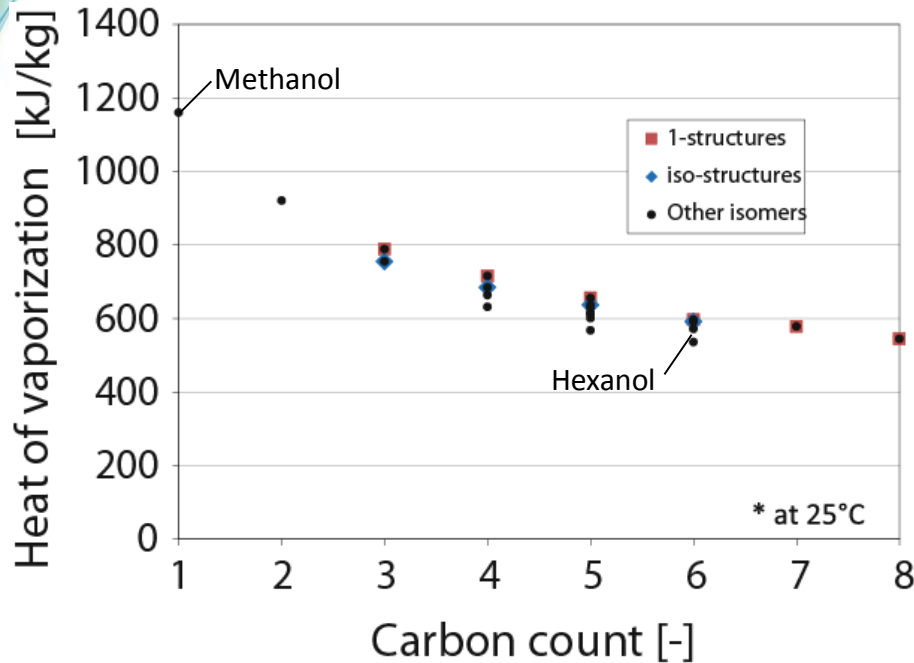
- But a large impact on KLSA is seen in DI engines (a measurable impact is seen at lower ethOH, too)

Several authors propose that HoV cooling can be represented by an “effective” RON increase

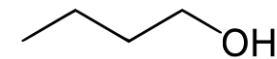
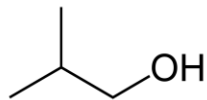
- Effective octane number increases of ~18 due to evaporative cooling have been found for E85
- The ~5 ON increase for E0 is inconsistent with some engine experiments, which show little difference in KLSA
- A more modest RON enhancement of:
 $0.16 * (\text{ethOH}\% - 40)$
 for ethOH blends above 40% has been suggested Leone, et al. , submitted
- A fuel-independent metric based directly on HoV would be desirable



Both the HoV and ON decrease for the higher alcohols



- Given the lower stoichiometric F/A ratio of the higher alcohols, and their lower HoV, little ON benefit is expected for moderate blend ratios
- Iso-structures generally have higher RON/MON than n- (or 1-) structures





HoV may have additional impacts not captured by “effective ON”

- Additional potential impact of HoV on efficiency SAE 2013-01-1634
 - Reduced heat transfer (~0.5% due to HoV)
 - Increased pumping work (lower MAP due to charge cooling, -0.3%)
 - Bookkeeping (impact of HoV on LHV results in artificially high BTE, +2.0%)

Overall, might expect an additional improvement in thermal efficiency of ~1% for every increment of 250 KJ/kg in HoV over gasoline



Phase change properties – distillation curve

D4814 –Specification for Automotive SI Fuel

- Imposes restrictions on:
 - The maximum vapor pressure at 100^oF (driven by emissions, lower than is required for vapor lock protection)
 - Maximum T_{10} (ensures sufficient low-T vaporization)
 - Maximum & minimum T_{50} (affects drivability and idling)
 - Maximum T_{90} / EP (affects oil dilution, correlates modestly with soot, may impact pre-ignition)
 - Maximum driveability index (typically < 590^oC):

$$DI = 1.5 * T_{10} + 3.0 * T_{50} + 1.0 * T_{90} + 1.33^{\circ} C * \text{ethOH}[\text{vol. \%}]$$

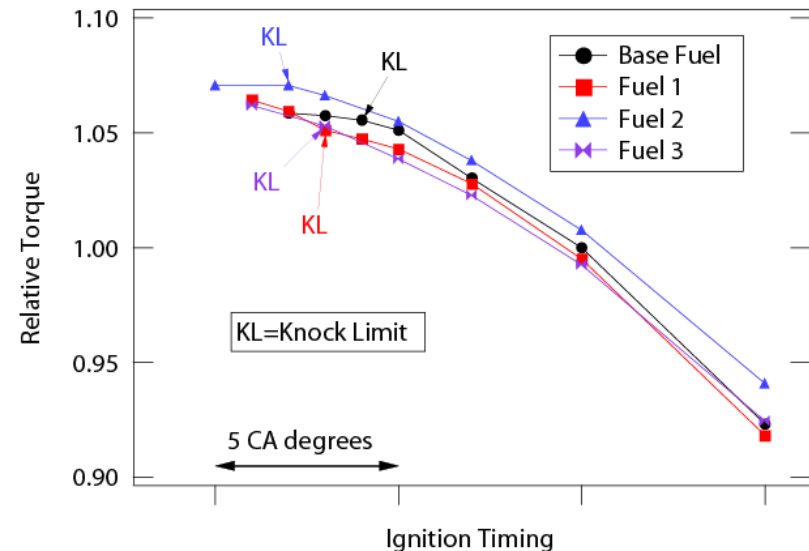
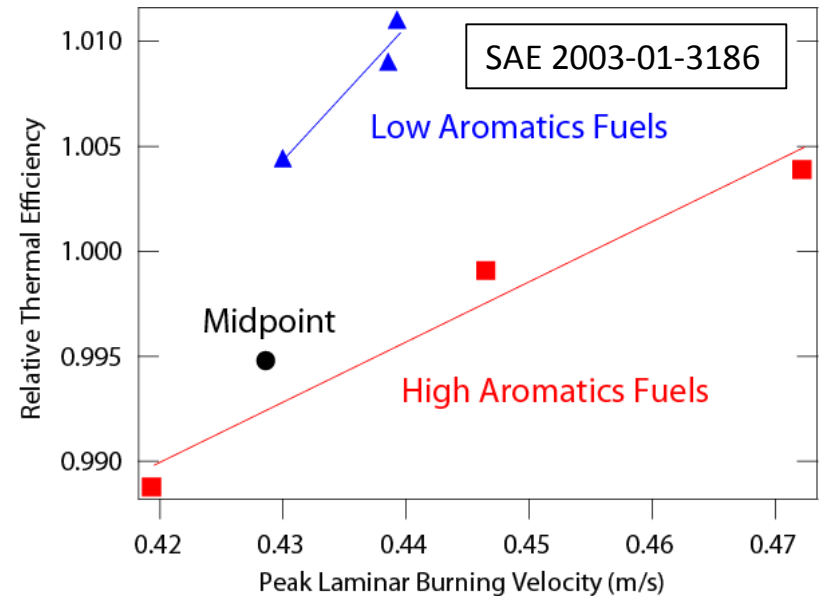
(ensures sufficient low-T vaporization, variation requires complex controls)

Flame speed can also impact efficiency

- Both vehicle and engine tests show that high flame speed fuels (high olefin, low aromatics) can increase efficiency by ~2%

See also Remmert, et al., 23rd Aachen Colloquim

- High flame speeds help mitigate knock and allow spark timing advance
- Flame speed may be particularly important for future lean burn engines (correlates with dilution tolerance)
- Benefits of high flame speed are more pronounced with higher EGR rates





High flame speed fuels are more susceptible to pre-ignition

- Pre-ignition is a two-step process
 - Ignition from surface, oil droplet, particle
 - Development of a flame kernel with a critical radius $\sim \delta$ (the flame thickness)

$$\delta = \left(\frac{\mu_0}{\rho_0 S_{l_0}} \right) \left(\frac{P}{P_0} \right)^{\sim -0.8} \left(\frac{T}{T_0} \right)^{\sim \pm 0.6}$$

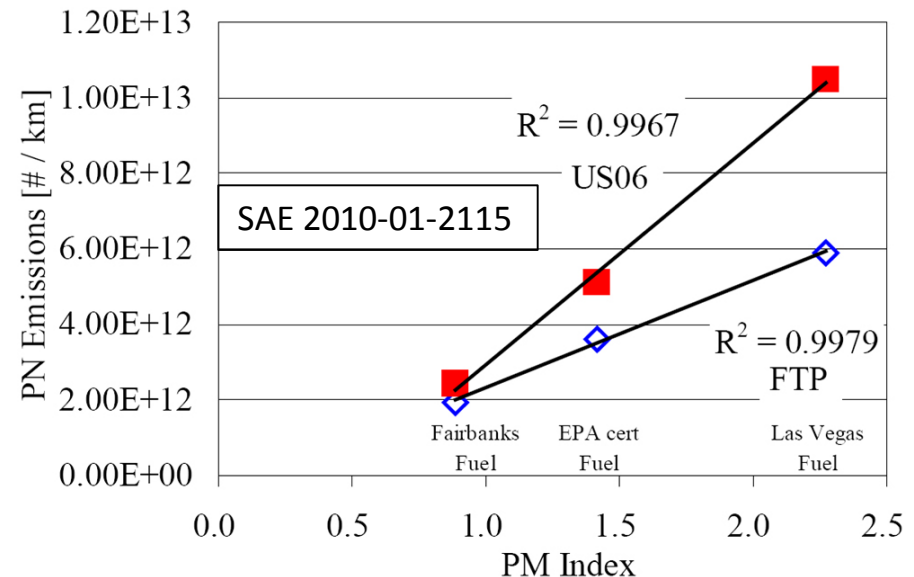
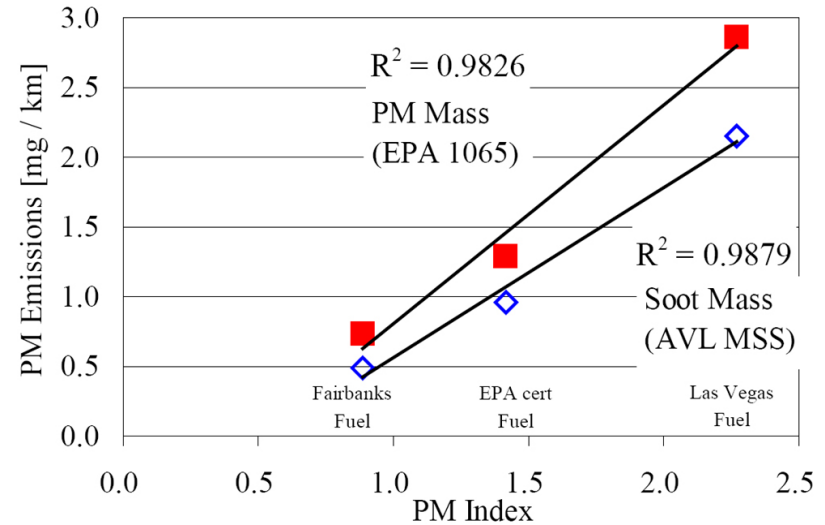
Does fuel sooting propensity impact efficiency? (Yes, if it necessitates a particulate filter)

- Soot mass and number seems to be well-correlated by:

$$PM\ Index = \sum_{i=1}^n I_{[443K]} = \sum_{i=1}^n \left(\frac{DBE_i + 1}{V.P(443K)_i} \times Wt_i \right)$$

$$DBE = \frac{(2C + 2 - H + N)}{2}$$

- Variation in PMI among commercially available fuels could give 10X variations in PM
- Additional data needed to draw firm conclusions





What fuel efficiency gains are possible with SI engine/fuel co-optimization?

- Baseline estimate (NA): (94/86 BOB + 15% ethOH)

- RON 91 → 100 (6.2%)
- Sensitivity 8 → 12 (MON 83 → 88) (1.4%)
- ΔH_{oV} 350 KJ/Kg → 85 KJ/Kg (0.3%)
- Flame speed 0.43 → 0.46 m/s (1%)

$$\Delta\eta = 9\%$$

- Optimistic estimate (NA): (98/86 BOB + 30% ethOH)

- RON 91 → 105 (9.7%)
- Sensitivity 8 → 16 (MON 83 → 89) (2.8%)
- ΔH_{oV} → 195 KJ/Kg (0.8%)
- Flame speed 0.43 → 0.46 m/s (1%)

$$\Delta\eta = 14.3\%$$

Additional benefits possible with lean combustion



SI Technologies: Legacy fleet efficiency gains

“In vehicle studies, many variables such as spark timing and fuel enrichment, transmission shift points, and others were calibration-dependent and therefore largely uncontrolled in these studies. Hence, the relationships between vehicle efficiency (fuel economy) and octane number could not be derived in any consistent manner from these vehicle studies”

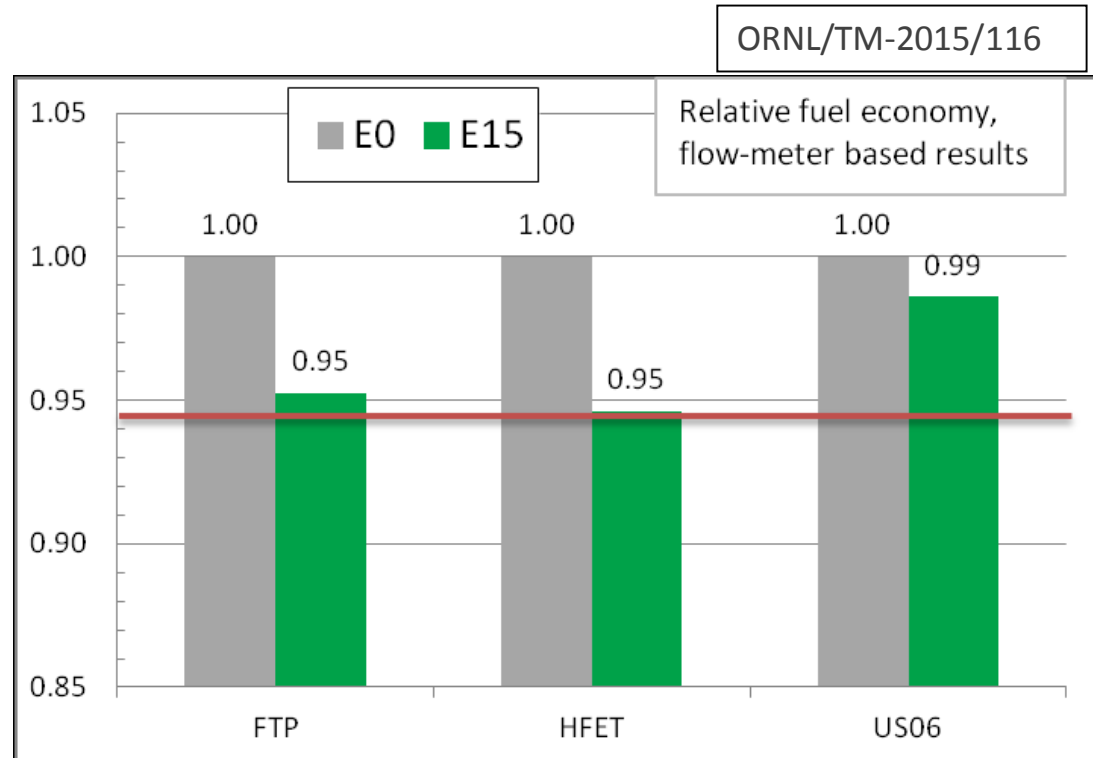
CRC CM-137-11-1b (2012)

- Little or no impact of ON on efficiency is expected if the engine is not knock-limited
- Recent tests on modern PFI and GDI engines showed FE changes largely proportional to fuel heating value when run on E30
- Performance benefits were seen on 3 of 4 vehicles tested, which could provide a driver for higher ON fuel sales

ORNL/TM-2015/116

Better legacy fleet efficiency gains are expected for down-sized or re-flashed engines

- Red bar represents TE parity. Note improvement under more aggressive driving.
 - E15 gives RON of 97.8
 - Downsized TDI 1 liter engine



- A recent study suggests that with ECU re-flashing, legacy fleet fuel economy gains for RON 91→97 range from 0.6% (light-load cycle, light vehicle) to 4.4% (aggressive cycle, heavy vehicle)



Research needs: Industry

- Better understanding of how ONR varies with r_c , considering bore size effects, speed effects, etc., & employing consistent engine design practices to maintain near optimal performance
- Need understanding of how the efficiency gain with increased r_c varies as bore size and application (drive-cycle) varies
- A more careful exposition of the extent to which downsizing / downspeaking can leverage compression ratio driven efficiency increases is needed
- Careful studies of fuel impacts on legacy vehicle fuel economy (w/ or w/o re-flashing)

The public domain data are insufficient to draw firm conclusions to guide policy makers/regulators, or to make a compelling case for a coherent, low GHG national transportation energy policy



Research needs: Universities and Labs

- Fundamentals of LTHR and HTHR for various fuel types:
 - Interactions with alcohols or other renewable blendstocks
 - Pressure dependencies
 - New metric for fuel autoignition, related to RON/MON
- Relating fuel properties to pre-ignition phenomena (T90, flame speed, etc.)
- Impact of HoV on performance or “effective ON”
 - Separation of chemical from thermal ON effects
 - Impact on heat transfer
 - Other potential efficiency impacts
- Develop a better understanding of how ONR & K varies over the engine map (provide clarity on minimum acceptable MON)
- Potential synergies between higher ON fuels and EGR



Research needs: Universities and Labs

- Blending studies to better characterize blend distillation characteristics, sooting propensities
- Impact of distillation curves on pre-ignition, oil dilution, soot (data must exist within the OEMs, possibly in the controls literature)
- How fuel properties impacting flame speed influence sooting propensity, distillation curves, ignition energies, flammability limits, pre-ignition propensity
- Additional studies on how fuel properties impact soot: soot inception and formation, bulk gas oxidation, PM trap oxidation
- Development of predictive simulation capabilities
- Lean combustion strategies (homogeneous & stratified)