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## LITERATURE REVIEW OF ETHANOL USE FOR HIGH OCTANE FUELS

## FINAL REPORT

Prepared for:

## **Renewable Fuels Association**

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#### **EXECUTIVE SUMMARY**

A literature review was performed to provide an objective view of the existing body of research regarding the use of ethanol to produce high octane gasolines in the US and the impact of high octane fuels on modern spark-ignited engine efficiency. The review found that ethanol has several innate characteristics that make it amenable to increasing the compression ratio and therefore the efficiency of modern spark-ignited engines. Ethanol has lower energy content than gasoline on a per-gallon basis. However, when ethanol is splash blended to increase the octane rating of the finished gasoline, and advantage is taken of the higher octane by increasing the compression ratio of the engine, mid-level ethanol blends can offer similar fuel economy and driving range as gasoline.

High octane, mid-level blends of ethanol ranging from 15-40% by volume are seen as offering the best trade-off between greenhouse gas (GHG) benefits and ease of implementation of fuel dispensing to achieve widespread availability. The National Renewal Energy Laboratory (NREL) concluded that since the UL already has a certification class for E25 dispensing equipment that is similar in price to E10 equipment, it would be the easiest to deploy and least costly of the high octane fuels.

Ethanol is known to have a high octane rating of approximately 108 research octane number (RON), giving it a high resistance to engine knock. For comparison, regular grade E10 gasoline has RON values typically around 92 for most of the US. What is less well-known, however, is that ethanol also has high sensitivity, meaning that in today's high power density engines, which often run with retarded combustion timing, the performance level can be extended to a greater degree than is indicated by RON alone. Ethanol also has a heat of vaporization that is almost four times higher than gasoline when compared on a stoichiometric combustion air basis. This means that in direct injection engines, there is a charge cooling effect giving ethanol a "cooling octane number" that is additive to it's chemical octane rating. The energy density of ethanol, on the other hand, is lower than that of gasoline on a volumetric basis so that one gallon of E85 fuel typically has about the same energy as 0.75 gallons of gasoline without any ethanol.

Numerous studies and technical papers from a wide variety of sources were examined for this literature review. A detailed bibliography of the studies reviewed is included with this report. The results from the studies reviewed generally support a main conclusion that splash blending ethanol is a highly effective means of raising the octane rating of gasoline and enabling low-cost efficiencies and reduced emissions in modern spark-ignition engines. For example, one study from an authoritative group of Original Equipment Manufacturers (OEM) scientists found that compression ratio increases leading to efficiency improvements of 5% for DI boosted gasoline engines could result from increasing the octane rating to 98 RON with 25% ethanol fuel. On the subject of emissions



impacts, one study noted GHG reductions of 6 – 9% depending on driving behavior with 98-RON E30 fuel at equal performance levels in engines having compression ratio raised from 10:1 to 13:1. On the economics of high octane fuels, one study found that the refinery cost of increasing octane to 98 RON from 93 RON is only \$0.02/gallon when ethanol is used as the means of increasing octane rating; however, the cost is \$0.20 gallon when hydrocarbon octane sources are used. Finally, one group used EPA's OMEGA tool for modeling the costs of achieving GHG standards for the 2025 model year and found that by adopting a 98 RON E25 fuel standard and increasing engine efficiency could result in a national cost savings of \$7B or a per vehicle savings of \$436 over continued use of regular E10 gasoline.



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## LITERATURE REVIEW OF ETHANOL USE FOR HIGH OCTANE FUELS

## 1 Introduction

The Renewable Fuels Association (RFA) has requested Ricardo to provide an objective review of the existing body of research concerning the technical merits of using ethanol as a blendstock to increase the octane rating of gasoline motor fuels sold in the United States. Furthermore, the Association is seeking a review of literature that examines how modern engine efficiency is impacted by the properties of ethanol-gasoline blends including the fuel's octane rating, the heat of vaporization and the sensitivity of the fuel or the difference between it's research octane number (RON) and motor octane number (MON).

Ricardo will expand upon and update the review that was performed last year in preparation for the RFA to submit comments on the EPA's Technical Assessment Report. This report embodies a new objective literature review articulating the technical issues regarding renewable fuels use in spark-ignited engines and motor vehicles. The report will examine in particular the effects on engine efficiency and performance through varying the fuel anti-knock index (RON + MON)/2, sensitivity (RON - MON) and the heat of vaporization.

# 2 APPROACHES TO IMPROVING VEHICLE FUEL ECONOMY AND ENGINE EFFICIENCY

Two main solution pathways to improving vehicle fuel economy and reducing CO<sub>2</sub> emissions have been outlined as the dominant approaches worldwide in recent years:

- High-efficiency naturally-aspirated engines utilizing high compression ratio, modified inlet valve closing strategies, and/or cooled exhaust gas recirculation, for high efficiency at lower specific rating
- Highly-boosted, downsized engines for part-load efficiency with relatively high specific rating

The Magma concept described by Osborne (Osborne, et al. 2017) represents an attempt to combine high compression ratio and advanced valve-timing strategy with downsizing and boosting in a Miller cycle with advanced boosting strategies to obtain greater efficiency benefits without compromising full-load performance.

Another main solution pathway is the hybridization of conventional internal combustion engines. This approach to improving vehicle and engine efficiency starts with simple engine start/stop strategies to reduce the amount of time the engine is idling and increases the amount of electric assist in an attempt to reduce the amount of time the engine is running



at low loads and make a shift towards operation at or near its peak efficiency point. Another added benefit of electrification is the ability to recapture the vehicle's kinetic energy instead of wasting it producing heat. The hybridization approach is often combined with the first main approach of increasing the efficiency of naturally-aspirated engines by increasing the compression ratio and modifying the inlet valve closing event to minimize the pumping work at the lower loads, often called Atkinson cycle. In recent years, Atkinson cycle engines have also been implemented in non-hybrid vehicles, albeit with not as great an increase in compression ratio nor modification of inlet valve closing timing, such as the Mazda Atkinson-cycle engine (Weissler 2011).

One more solution pathway to increasing efficiency is variable compression ratio, wherein the engine operates at high compression ratio at lower loads and switches to a lower compression ratio when high loads are called for. Variable compression ratio (VCR) has been researched for years (Boretti, Scalzo and Masudi 2011) with many different mechanisms being investigated but has only recently been developed to the point of production-intent by Nissan Motor Co. (INFINITI 2017), (autoblog 2016). The fuel economy benefits of 2-step and continuously variable VCR was examined by Shelby (Shelby 2017). The study estimated a 2-step VCR fuel economy benefit of 2.5-3.1% on the EPA metrohighway (M-H) drive cycle and 0.8-1.2% on the US06 cycle relative to a fixed 10:1 compression ratio engine. The benefit levels increased slightly for continuously variable VCR compared to 2-step to 2.7-3.3% on the M-H and more significantly on the US06 to 1.7-2.1%.

There are two key, fundamental mechanisms being addressed by the solution pathways outlined above: firstly, the compression ratio which at the most basic level controls the overall thermodynamic effiency of an engine cycle and secondly, the parasitic losses in an engine which limit the amount of useful shaft power that can be produced from the conversion of the fuel's energy into heat. The parasitic losses can be further broken down into mechanical friction and pumping loss or engine breathing losses. Mechanical friction is mainly dependent on engine speed but pumping losses are mainly dependent upon engine load with higher losses being incurred at lower loads due to throttling as the primary means for controlling engine load in a spark-ignited (SI) engine. Pumping losses can be minimized through either early intake valve closure (EIVC) or late intake valve closure (LIVC) approaches for stoichiometric engines or by lean operation. There are challenges to keeping emissions in check with lean combustion systems and these approaches require lean NOx aftertreatment; nonetheless these technologies are showing promise in also achieving cost reductions as they continue to be developed.

The optimal intake valve closure strategy has also been the subject of debate and research for some time (Boggs, Hilbert and Schechter 1995) with various outcomes depending on



whether it is applied to a naturally-aspirated or a boosted engine (Ferrey, et al. 2014). Comparisons between EIVC and LIVC have recently been made experimentally on an SI engine with the EIVC strategy showing slightly greater potential to improve engine efficiency at part-load conditions, although both approaches were better than the conventional throttled approach (Lanzanova, Nora and Zhao 2017). The major drawback of the EIVC strategy was longer combustion duration, and it is for this reason that Osborne et al. use a modified intake port to enhance the tumble motion when adopting the EIVC strategy for the Magma concept.

## 3 LIMITATIONS ON EFFICIENCY IMPROVEMENT

There are practical limitations to improving the efficiency of modern gasoline engines that fall into two categories: structural limitations and end-user acceptability limits. Structural limitations define the peak pressures within the cylinder and maximum material temperatures that can be tolerated. There are also limitations that come about from a vehicle user's desire for comfort, namely the noise, vibration and harshness (NVH) experienced in the vehicle. These vehicle characteristics have been translated into engineering requirements on the engine in the form of limits on the rate of pressure rise and on the variation of average pressure over an engine cycle. Rate of pressure rise impacts the sound quality and harshness of sound that is emanating from the engine and the variation of average pressure has to do with the lower frequency vibrations that are transmitted through the vehicle structure and felt by the driver. Rate of pressure rise will be discussed more in the section on engine knock.

The average pressure over an engine cycle is known as the mean effective pressure (MEP) and is used as a measure of the work produced per cycle. Variation of MEP represents the variation in work output from cycle to cycle and the coefficient of variation (COV) is therefore a measure of variability of work produced expressed as a percentage of the average work per cycle. The COV of IMEP then is used as a measure of the variation of work output or strength of combustion. The "I" before MEP simply means that it is *indicated* from the cylinder pressure diagram and is the maximum work that can be done by the combustion pressures acting on the piston top before friction and pumping losses are subtracted.

There are two ways of expressing the IMEP for a 4-stroke engine: gross IMEP and net IMEP. Gross IMEP is calculated as the mean cylinder pressure averaged over all four strokes of the cycle including the intake and exhaust breathing strokes; net IMEP, or NMEP for short, is the mean pressure calculated only over the compression and expansion strokes of a combustion cycle, and is therefore a purer measure of the work obtained from combustion without reference to the intake and exhaust strokes. For this reason the COV of IMEP is



sometimes referred to as "combustion variability." In either case, variation in IMEP is a key component of the forcing function for the vibrations that are felt in a vehicle and are especially noticeable at idle conditions where the average IMEP is small. Limits are set during engine testing programs for the COV of IMEP at 3% or less typically which represents an acceptable level of combustion variation that is derived from studies of what drivers perceive as tolerable levels of vibration within a vehicle.

## 3.1 Engine Knock

The most common phenomenon limiting gasoline engine performance and efficiency is commonly known as knock which tests all of the limiting design factors and can result in severe engine damage if not properly controlled. The engine structure can be stressed well-beyond design limits due to the very high cylinder pressures that are created with severe knock. The fact that knock is a very fast, localized heat release means that pressure waves are generated and can lead to very high heat transfer rates from the scrubbing action of the waves raising combustion chamber surface temperatures if it is prolonged. The fast heat release gives rise to pressure waves in the cylinder that are in the audible frequency range which excite the engine structure with a characteristic knocking sound. The audible knocking frequency range is much higher (as shown below by Naber (Naber, et al. 2006) in the section on knock measurement) than the low frequency COV of IMEP variations described above which are felt as vibrations in a vehicle.

The theory behind knock was described by Draper (Draper 1933) in a NACA report as follows: "If a firecracker is exploded inside a closed drum containing air, two effects naturally follow: A series of sound waves is set up by the sudden local increase in pressure at the explosion and the general pressure within the drum rises because of the energy liberated. The frequency of the resulting sound waves will depend on the dimensions of the drum, the air pressure, and the position of the firecracker within the drum. It is reasonable to suppose that the process known as detonation in internal-combustion engines is similar to that taking place in the case outlined above." Draper further developed the theory of knock in order to quantify its characteristics as illustrated in Figure 1.



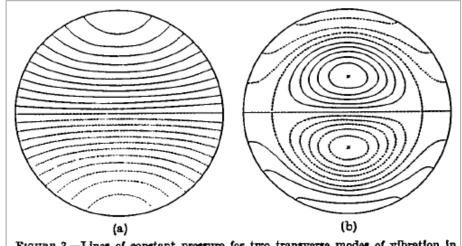


FIGURE 3.—Lines of constant pressure for two transverse modes of vibration in circular cylinder: (a) Single nodal plane; (b) one nodal cylinder in addition to nodal plane.

FIGURE 1 PRESSURE WAVE PATTERNS IN A CYLINDER AS DESCRIBED BY DRAPER



Heywood (Heywood 1988, 462) described knock as emanating from "autoignition of the fuel-air mixture in the end-gas. *Autoignition* is the term used for a rapid combustion reaction which is not initiated by any external ignition source." Naber have used both cylinder pressure transducers and accelerometers mounted on an engine block to compare alternative ways of measuring and controlling knock. Figure 2 compares the cylinder pressure traces and the band-pass filtered signals (5-27 kHz) which were used to determine knock intensity. The frequencies of the filtered pressure signals correlates well with the modes of vibration originally developed by Draper. The knocking intensity was also quantified by Naber's measurements and expressed as a pressure intensity for the amplitude of the filtered pressure signal or an accelerometer intensity based on the filtered accelerometer signal.

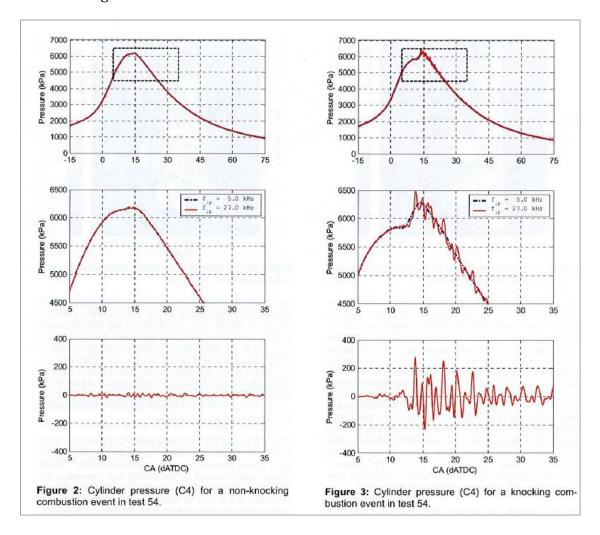


FIGURE 2 CYLINDER PRESSURE TRACES FROM NON-KNOCKING (LEFT) AND KNOCKING (RIGHT) COMBUSTION EVENTS. (FROM NABER)



## 3.2 Low-speed pre-ignition and mega-knock

Low-speed pre-ignition (LSPI) is another phenomenon related to to knock and occurs when enough heat is released before the spark can initiate a normal combustion event. LSPI can lead to mega-knock that can quickly destroy an engine; the results of low-speed pre-ignition and mega-knock can be seen in the piston damage shown in Figure 3 from Mayer (Mayer, Hofmann and Williams, et al. 2016a)



FIGURE 3 PISTON DAMAGE OCCURRING AS THE RESULT OF LOW-SPEED PRE-IGNITION LEADING TO MEGA-KNOCK (FROM MAYER, 2016A)

The pre-ignition event, deflagration of the flame that was initiated by the spark, and mega-knock are all apparent in the pressure diagrams shown in Figure 4. There are multiple causes for LSPI such as detached combustion chamber deposits or hot residual gas but this work undertakes developing a methodology to verify only oil induced pre-ignitions. Mayer, 2016a clearly demonstrates that calcium detergent additives in engine oils were able to induce self ignitions whereas magnesium detergents failed to reach its critical temperature, as shown in Figure 5.



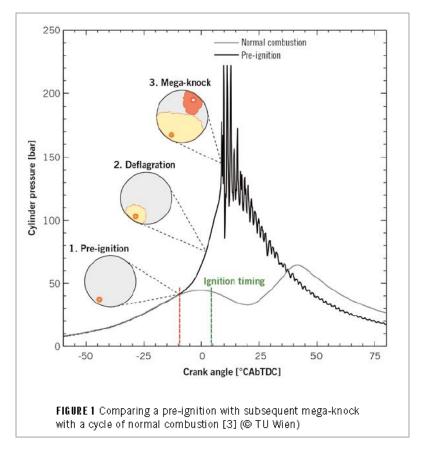


FIGURE 4 PRE-IGNITION LEADING TO MEGA-KNOCK AS SHOWN BY MAYER, 2016A

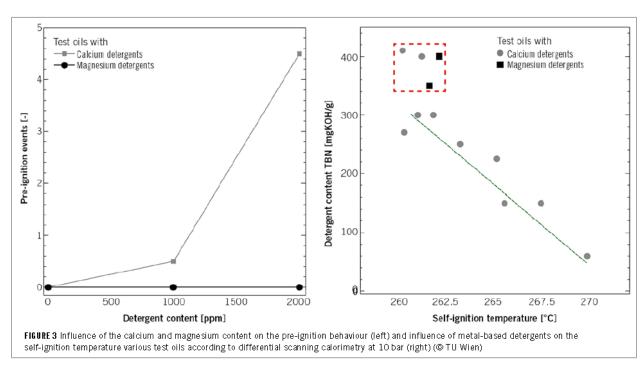


FIGURE 5 PRE-IGNITIONS CAUSED BY CALCIUM DETERGENTS BUT NOT BY MAGNESIUM DETERGENTS (FROM MAYER, 2016A)



In a study on using enrichment with a DI injector with charge cooling to suppress very heavy knock levels (up to 40 bar), a trade-off was observed in which knock intensity first increased by up to 60% before lower unburned gas temperatures suppressed knock under extremely rich conditions (vafamehr, Cairns and Moslemin Koupaie 2017). Such a trade-off is not usually observed in low-to-moderate knock intensity situations. The trade-off was associated with reducing auto-ignition delay times outweighing increasing charge cooling and ratio of specific heats. Ethanol was seen to be more effective than other fuels in reducing knock intensity. Overall, the results demonstrate the risks in employing excess fuel to suppress knock deep within a heavily knocking combustion regime (potentially including a super-knock regime).

## 3.3 Testing limits imposed by knock

The limitations on efficiency improvement, both structural and user acceptability limits, have been well understood and translated into engine-specific engineering criteria so that engines can be tested in a repeatable manner on an engine dynamometer. Test procedures have been applied to determine the peak torque that can be achieved from an engine using different fuels. The basis of these test procedures is to identify the borderline knocking condition, that is the engine operating conditions where knock first becomes robustly detectable; an engine is operating at knock-limited conditions when borderline knock is detected. Test procedures such as these have been rigorously applied and are described in the following description adapted from Stein et al (Stein, Polovina, et al. 2012).

Starting from a low load point and as inlet pressure and NMEP are increased, the engine becomes more knock-limited and spark timing must be retarded. As NMEP increases and combustion phasing is retarded, the exhaust temperature increases both due to the higher load, which reduces heat transfer per unit mass, and due to degraded efficiency, which results in increased energy in the exhaust gas. When exhaust gas temperature reaches its limit, lambda (defined as the air-fuel ratio divided by the stoichiometric air-fuel ratio) must be enriched to control exhaust temperature. Although turbocharged SI engines typically have a 950°C turbine inlet temperature limit, it was found from experience that an exhaust temperature of 850°C on the single cylinder engine used in these tests corresponded to a multi-cylinder engine exhaust temperature of 950°C. Finally, as inlet pressure and NMEP are further increased, the peak cylinder pressure can also increase, depending on the amount of combustion phasing retard. Once the peak cylinder pressure reaches the engine's structural limit, the spark timing must be retarded. A load sweep wherein these test procedures were applied and the specific limits for each constraining parameter is illustrated in Figure 6. In the top graph CA50 indicates the crank angle (CA) where 50% of the fuel is burned, representing the mid-point of combustion, and was set at 30° aTDC (after top dead center) as combustion stability tends to become unstable beyond that. In



the third graph from the top lambda is ideally equal to 1.0, except as needed to protect the exhaust turbine.

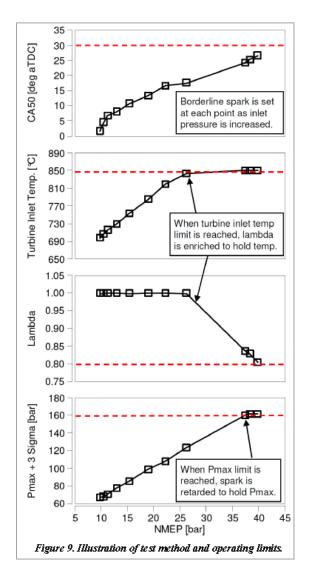


FIGURE 6 APPLICATION OF TEST PROCEDURES AND LIMITS ON ENGINE PERFORMANCE (FROM STEIN, 2012)

## 4 FUEL PROPERTIES

# 4.1 Octane and anti-knock ratings

Because engine knock is such a dominant factor in limiting the efficiency and performance of modern gasoline engines, it is important to understand the characteristics of fuels as they strongly influence the knocking tendency of SI engines. The tendency of gasoline fuels to resist knocking in an engine is known as the octane number. "Octane number is not a single-valued quantity and may vary considerably depending on engine design, operating



conditions ..., ambient weather conditions ..., mechanical condition of engine, and type of oil and fuel used in past operation. ...Several octane rating methods have been developed. Two of these - the research method (ASTM D-2699)¹ and the motor method (ASTM D-2700) - are carried out in a standardized single-cylinder engine" (Heywood 1988, 471) under two specified sets of engine operating conditions giving a research octane number (RON) rating to a fuel, and a motor octane number (MON) rating to a fuel, respectively. The anti-knock index (AKI) then is the arithmetic average of the RON and MON numbers.

It is important to understand the engine operating conditions for the RON and MON tests so applicability to today's engines can be assessed. The RON and MON tests are both done in a variable compression ratio single-cylinder engine known as a "Cooperative Fuel Research (CFR<sup>TM</sup>) engine manufactured by GE Energy Waukesha,"<sup>2</sup> (Stein, Polovina, et al. 2012) but at different inlet conditions, engine speeds and spark timings as shown in Table 1.

TABLE 1 FROM STEIN, 2012

Table 1. Engine conditions for the RON and MON tests.

Parameter	RON	MON	
Inlet Air Temperature	52℃	38℃	
Inlet Mixture Temperature	*	149℃	
Intake Air Pressure	atmospheric	atmospheric	
Coolant Temperature	100℃	100℃	
Engine Speed	600 rpm	900 rpm	
Spark Timing	13° bTDC	14 - 26° bTDC	
Compression Ratio	4 - 18	4 - 18	

<sup>\*</sup>Not specified, but will be lower than the inlet air temperature.

"Carburetion is used for fuel introduction in these tests. For the RON test, the inlet air temperature of 52°C is set upstream of the carburetor." (Stein, Polovina, et al. 2012) As a consequence the RON test more closely mimics the conditions of a port-injected engine where the fuel evaporation cools the fresh charge mixture in the intake port. "For the MON test, the inlet air-fuel mixture temperature of 149°C is set downstream of the carburetor." (Stein, Polovina, et al. 2012) Consequently the MON test does not include any of the charge cooling effect from the fuel evaporation. That is why "many published papers ... indicate that the knock resistance of a fuel in modern engines more closely realtes to RON." (Stein, Polovina, et al. 2012) In direct injection (DI) engines, however, all of the fuel evaporation takes place within the cylinder, although much of the heat of vaporization may be picked up from the combustion chamber walls rather than the air charge for wall-guided injection

 $<sup>^{1}</sup>$  ASTM denotes American Society for Testing and Materials; the letter and number defines the specific testing code.

<sup>&</sup>lt;sup>2</sup> The CFR engine manufacturing rights have been owned by CFR Engines, Inc. since 2014.



systems. Regardless of the type of DI injection spray however, it is the cooling of the fresh air charge in the cylinder that enables an increase in the amount of charge that can be inducted and an increase in the resistance to knock.

Vertin (Vertin, et al. 2017) studied the effects of gasoline AKI at high altitude and found that vehicles operating with 85 AKI fuel showed strong evidence detected onset of knock earlier than when operating with 87 AKI fuel and used different engine control setting for knock avoidance. As a consequence they found all 5 of the tested vehicles showed some reduction in net power. Williams (Williams, et al. 2017) found that, for Euro 5 and Euro 6 passenger cars, the benefits of moving to higher octane fuel were about double on the US06 test cycle than those observed for the WLTC test cycle.

The octane index (OI) has been proposed as a better way to describe the anti-knock quality of gasolines in modern DI engines by Kalghatgi (Kalghatgi, Fuel/Engine Interactions 2013), (Kalghatgi, Head, et al. 2014) where

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

The fuel's sensitivity is the difference between its RON and MON ratings, or S = RON - MON, and the equation can be rewritten as

$$OI = RON - K * S$$

For downsized turbocharged engines running at higher torque levels, the values of K have been found to be negative; i.e. the anti-knock performance of a fuel increases proportionally with RON and with fuel sensitivity. However, Stein (Stein, 2012) noted the values of K depend on the operating conditions of the engine, the fuel system type, and the fuel's chemical knock resistance and heat of vaporization; K decreased with increasing evaporative charge cooling (e.g. as provided by DI fuel injection or higher ethanol concentration in the fuel) and with increasing combustion phasing retard, and K increased with increasing inlet temperature and increasing compression ratio. A recent study by Zhou (Zhou, et al. 2017) compared four different test methods for determining K. The value of K was found to be consistently negative at higher loads with DI. However, at part-load conditions, K was determined to approach 0.5.

# 4.2 Chemical octane and charge cooling effects

Recognizing not only the importance of a fuel's 'chemical' octane rating as expressed by its RON and its sensitivity, but also a fuel's heat of vaporization to further reduce the propensity to knock in DI engines, Stein, 2012 designed a set of experiments to cleanly separate the two effects. This was accomplished by comparing performance of a neat gasoline (E0) to an E50 blend made from the same 88 RON gasoline blendstock splash blended with 50 v% ethanol, first of all using an upstream fuel injection (UFI) system and



secondly with a DI injection system. Figure 7 shows the chemical octane effect by the difference between the red and green lines and the charge cooling effect by the difference between the blue and red lines. The chemical octane effect is seen by comparing the E50 blend to the E0 gasoline, with octane ratings of X and Y respectively, where both fuels were fully evaporated before entering the engine by UFI. The charge cooling effect is seen in this case by comparing the same E50 fuel as introduced directly into the cylinder, thereby utilizing the full heat of vaporization of the ethanol blend by DI injection for charge cooling, to introduction of the fuel upstream with UFI injection which has no charge cooling incylinder.

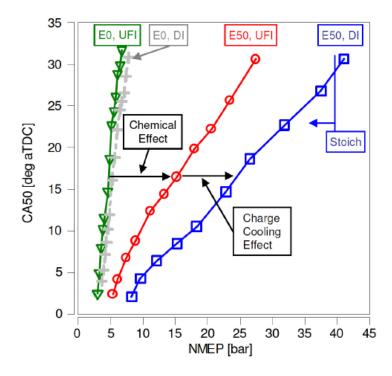


FIGURE 7 SEPARATION OF CHEMICAL OCTANE AND CHARGE COOLING EFFECTS (FROM STEIN, 2012)

As illustrated by the two black arrows at 16 deg aTDC CA50 timing, the maximum achievable NMEP at equal knock-limited combustion phasing increases from 5 bar to 15 bar solely due to the chemical octane increase and from 15 bar to 24 bar exclusively due to the influence of increased charge cooling.

# 4.3 Sensitivity to autoignition kinetics

A fuel's sensitivity (RON – MON) plays a profound role in its ability to resist knock and the anti-knock ability increases as combustion phasing is retarded from minimum spark advance for best torque (MBT). Mittal (Mittal, Heywood and Green 2010) explained that sensitivity is a measure of how much the autoignition kinetics of a fuel vary with the temperature of the unburned end gas, as shown in Figure 8. Note the logarithmic scale on



the y-axis to get a better sense of how much autoignition delay times can be impacted by temperature. Shorter delay times means the fuel-air mixture will reach it's critical autoignition point (i.e. knock) sooner. Figure 8 also shows conceptually how a high sensitivity fuel exhibits much longer autoignition delay times at low temperatures compared to a low sensitivity fuel and therefore a reduced tendency to knock. The conditions where high sensitivity fuels exhibit this tendency include the end gas temperatures in DI engines and turbocharged DI engines with retarded combustion phasing.

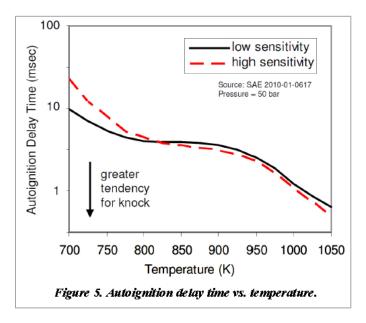
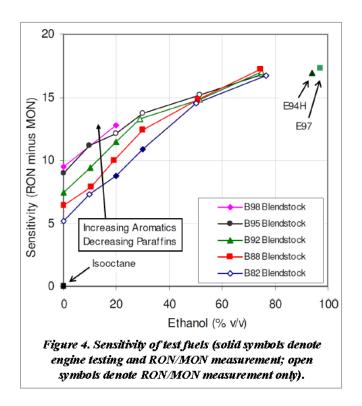


FIGURE 8 CONCEPTUAL ILLUSTRATION OF HIGH AND LOW SENSITIVITY FUELS KNOCKING TENDENCY (FROM STEIN, 2012)

The sensitivity of the fuels as ethanol is blended in increasing percentage is shown in Figure 9 with ethanol having a high sensitivity value greater than 15. As can be seen in Figure 7, above, the reduction in slope of the curves as combustion phasing (CA50) is retarded is due to the high sensitivity of the autoignition kinetics of ethanol to unburned gas temperature. The effect of ethanol's high sensitivity on the bending over of the CA50 vs NMEP curves is seen to a greater degree in Figure 10 with an E75 blend having an almost unlimited ability to resist knock as it's curves tend to level off at increasing NMEP levels while not having reached the 30° aTDC retard limit yet, except for the UFI case. Notice also how the E0 gasoline, with a much lower sensitivity, displays very little if any bending of it's curves.





### FIGURE 9 FUEL SENSITIVITY VS ETHANOL PERCENTAGE (FROM STEIN, 2012)

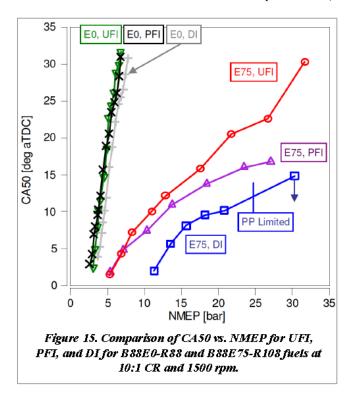


FIGURE 10 COMBUSTION PHASING VS NMEP FOR E0 AND THE E75 BLEND SHOWS GREATER BENDING OF THE CURVES THAN E50 (FROM STEIN, 2012)



A recent study using only E10 blends from Shell Global Solutions (Prakash, et al. 2017) also found that higher sensitivity fuels had a positive impact on engine thermal efficiency even though RON was more influential.

## 4.4 Fuel and oil impacts on pre-ignition and mega-knock

The influence of different ethanol fuels was investigated to analyze the effects of wall wetting in a DI engine on pre-ignitions (Mayer, Hofmann and Geringer, et al. 2016b) using the same methodology as outlined in Mayer, 2016a. In this study the fuel volatility was varied in order to change the amount of fuel impinging on the cylinder walls and mixing the oil film from the spray-guided DI fuel spray. They show that the number of pre-ignition events decreases up to 30~v% ethanol due to increasing heat of vaporization and charge cooling, but at 50~v% ethanol the rate of pre-ignition events rises drastically, Figure 11.

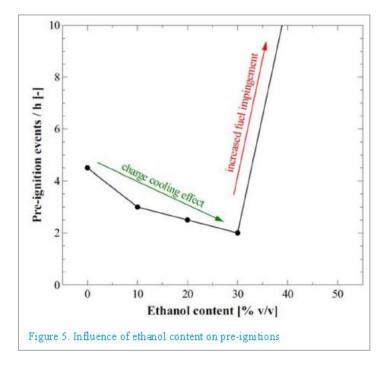


FIGURE 11 EFFECTS OF ETHANOL CONTENT ON RATE OF PRE-IGNITIONS (FROM MAYER, 2016B)

It is hypothesized and then demonstrated that the effect of increased fuel impingement overwhelms the increased charge cooling effect as seen in Figure 12. The "E50specE30" fuel is a blend of the E30 test fuel mixed with neat ethanol to bring it up to 50 v% ethanol, with similar volatility curves as E50. It is also noted that the tendency for mega-knock events is greatly reduced relative to the frequency of pre-ignition events due to increased charge cooling at higher ethanol concentrations.



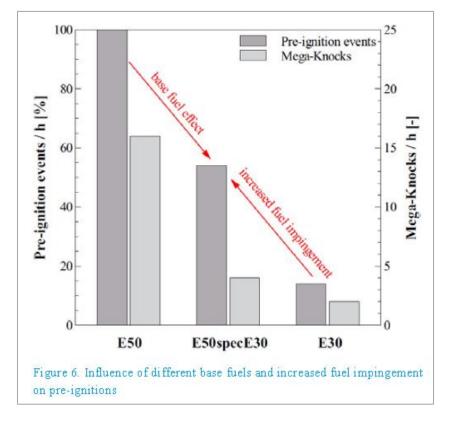


FIGURE 12 BASE FUEL AND FUEL IMPINGEMENT EFFECTS ON PRE-IGNITIONS (FROM MAYER, 2016B)

From these experiments and others, Mayer, 2016b develop a model for the amount of liquid fuel that evaporates from 150°C up to the final boiling point to correlate almost perfectly with the rate of pre-ignition events as shown in Figure 13, reinforcing the hypothesis that droplets formed by fuel-oil mixture can be a significant contributor to pre-ignition.



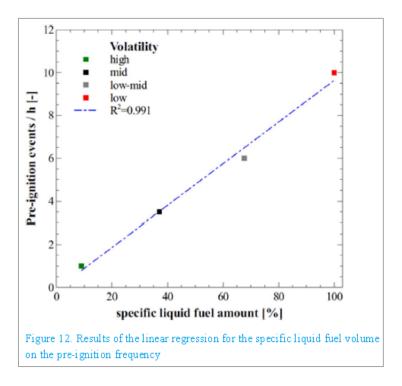


FIGURE 13 CORRELATION OF SPECIFIC FUEL VOLUME TO PRE-IGNITIONS (FROM MAYER, 2016B)

## 4.5 Fuel Effects on Tailpipe and Evaporative Emissions

Because of the rising use of ethanol around the 2007 timeframe, West (West, et al. 2007) acquired a Saab 9-5 flex fuel vehicle (FFV) that was certified to Euro 4 emissions. Taking advantage of ethanol's greater anti-knock properties, Saab specified the turbocharged engine at 180 hp on E85, 20% higher than the gasoline power rating of 150 hp. European emissions regulations required certification on gasoline only, however US regulations required certification on both gasoline and E85, so the vehicle was tested on both fuels. As can be seen in Figure 14 the vehicle showed significantly lower NMHC+NO<sub>x</sub> and CO emissions over the US06 test cycle when fueled with E85 than with gasoline. Stein (Stein, Anderson and Wallington, An Overview of the Effects of Ethanol-Gasoline Blends on SI Engine Performance, Fuel Efficiency, and Emissions 2013) note a CRC study (Haskew and Liberty 2011) which similarly found a statistically significant trend of decreasing NMHC and NMOG for US06. However there were no significant changes to tailpipe emissions noted on the other test cycles. Stein, 2013 also found lower PM emissions with increasing ethanol content.



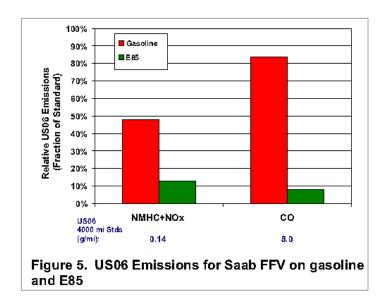


FIGURE 14 EMISSIONS COMPARISON OF AN FFV RUNNING ON GASOLINE AND E85 (FROM WEST)

The EPA regulates the vapor pressure of gasolines in order to limit the evaporative emissions from refueling and other sources on the vehicle. Ethanol-gasoline blends actually have the highest vapor pressure at 10 v% ethanol as shown in Figure 15. The EPA allows a "1 psi waiver" to E10 gasoline blends to encourage the blending of 10% ethanol in gasolines. Stein, 2013 notes that higher levels of ethanol are expected to have little impact on evaporative emissions in modern vehicles.

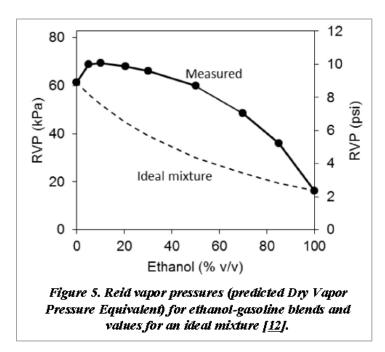


FIGURE 15 REID VAPOR PRESSURE PEAKS AROUND 10% ETHANOL (FROM STEIN, 2013)



## 5 SOLUTIONS TO TREATING THE ENGINE & FUEL AS A SYSTEM

## 5.1 Co-Optimization of Fuels & Engines (Co-Optima) Initiative

Transportation accounts for 70% of U.S. petroleum consumption and 27% of the country's greenhouse gas (GHG) emissions, and the internal combustion engines (ICEs) that generate most of these emissions will continue to power vehicles for decades to come. The U.S. Department of Energy's (DOE's) Co-Optima initiative is accelerating the introduction of affordable, scalable, and sustainable fuels and high-efficiency, low-emission engines with a first-of-its-kind effort to simultaneously tackle fuel and engine research and development (R&D) (DOE 2016).

The DOE has developed a 'merit function' in order to quantify the components of efficiency gain that can be expected from high octane fuels as used in high efficiency engines. "The merit function numerically represents the efficiency gain that can be expected compared to a "current market fuel"." (Miles 2016) The contributing factors to efficiency gain are: RON, Octane sensitivity, heat of vaporization, flame speed, distillation and particulate emissions as expressed in the equation of efficiency merit:

$$Merit = \sum \frac{\text{RON}}{1.6} - \frac{\text{Sensitivity}}{1.6} + \frac{(RON_{mix} - 91)}{1.6} - \frac{(RON_{mix} - 91)}{1.6} + \frac{(N_{mix} - 8)}{1.6} + \frac{(N_{mix} - 8)}{1.6} + \frac{(N_{mix} - 8)}{1.6} + \frac{(N_{mix} - 415[kJ/kg])}{1.6} + \frac{(N_{mix} - 415[k$$

The intent of the merit function is to provide a guide to the DOE research teams to address two important questions: what are the important properties and where should efforts be focused? However, there are stated limitations to what can be achieved by the research being performed under the guidance provided through the merit function however. Specifically, those limitations of the merit function are:

- Applicable only to stoichiometric SI engines
- Considerably simplified (e.g. does not distinguish between NA and turbocharged engines)
- Incomplete knowledge of the impact of many fuel properties (this is a major objective)
- Lack of knowledge of blending effects on properties
- Does not consider properties that do not impact efficiency (e.g. RVP)
- Property interactions have not been investigated thoroughly (e.g. RON & HoV)



• Estimates only an "average" efficiency increase (e.g. does not consider drive cycle effects or different vehicle applications)

Nonetheless, the merit function serves as a useful tool in assigning values to the various contributing factors of efficiency and guiding DOE research efforts. Co-Optima has also incorporated the viewpoints from multi-disciplinary stakeholder groups towards "accelerating the introduction of affordable, scalable, and sustainable fuels and high-efficiency, low-emission engines." Stakeholder groups participating in last year's workshop included trade/consumer groups, petroleum industry, original equipment manufacturers, and the biofuels industry.

## 5.2 Octane on Demand

Professor John Heywood and co-workers at MIT (Cohn, Bromberg and Heywood 2005) first published the idea of using a high octane fuel such as ethanol only as needed to suppress knock while using a lower octane fuel for the rest of a vehicle's needs in 2005. Their approach involved injecting ethanol directly into the cylinder at high loads for knock suppression and increasing the compression ratio to increase the efficiency of the engine at all operating conditions. The engine would run on gasoline at lower loads where knocking was not present which represents a majority of the time for average driving behaviors. Thus, a small amount of ethanol use was "leveraged" into a much greater savings of gasoline, to the tune of a 30% reduction in overall  $CO_2$  emissions from the gasoline efficiency savings combined with the lower  $CO_2$  from substituting ethanol for gasoline.

The concept of leveraging high-octane ethanol into a greater reduction of gasoline use was applied by Stein (Stein, House and Leone, Optimal Use of E85 in a Turbocharged Direct Injection Engine 2009) to a Ford Motor Company EcoBoost® engine. The engine was modified by adding a PFI system to the DI engine as shown in Figure 16 and by increasing compression ratio to 12:1.



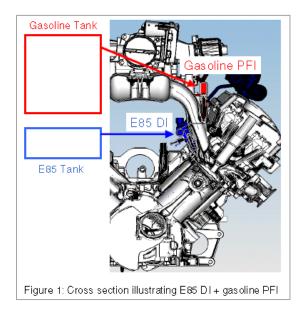


FIGURE 16 ETHANOL LEVERAGING OF GASOLINE ON A FORD ECOBOOST V6 ENGINE (FROM STEIN, 2009)

With the results from testing the engine on a dynamometer they simulated in an F150 pickup truck how much E85 would be required for various drive cycles and overall fuel consumption. The study found that only 1% of the total fuel mass was required from E85 on mild drive cycles like the EPA metro-highway (M-H) test cycle, and 16% on more aggressive US06 driving. However, on the very heavily-loaded scenario of driving up the Davis Dam road in Arizona for 10 miles with a fully loaded vehicle and trailer at it's gross combined weight rating (GCWR) required nearly half the fuel mass to come from E85.

TABLE 2 E85 USE FOR VARIOUS DRIVE CYCLES AND LOADING CONDITIONS (FROM STEIN, 2009)

fuel n	Table 3: Modeled E85 consumption as a percent of total fuel mass for a 5.0L E85 DT+ gasoline PFI engine in a pickup truck							
		at ETW	at GCWR					
	EPA City	1%	19%					
	EPA Highway	1%	30%					
	US06	16%	-					
	Davis Dam	-	48%					

This concept is an example of what has been called "octane on demand." While ocatane on demand offers a technically superior solution in terms of  $CO_2$  emissions savings and oil consumption reduction, it has the obvious drawbacks of needing two tanks of fuel on board and requiring vehicle drivers to fill the tanks with two different fuels.



## 5.3 Higher Octane Floor for US Regular Gasoline

In marked contrast to the octane on demand approach which may be technically superior but has onerous requirements of vehicle operators, there is another approach to improving efficiency and reducing GHG emissions by treating the engine and fuel as a system that is being talked about more openly by automotive OEM executives. That approach makes use of the vehicle efficiency gains stemming from higher octane fuels and moves the onus from the vehicle operator to other stakeholder groups, as seen in part by participation in Co-Optima's workshops:

- petroleum refining
- biofuels industry
- gasoline retailing

In addition to these stakeholder groups needing to undertake changes to their business operations, the United States government would need to regulate (through the EPA), the changes to the gasoline fuels that would be required for use in future vehicles.

Increasing the octane floor of regular grade gasoline sold across the US in order to take advantage of efficiency gains would require the petroleum refining industry to maintain existing octane ratings of their gasoline blendstocks, as noted by Hirshfeld (Hirshfeld, et al. 2014). Leone (Leone, Anderson, et al. 2015) found that higher octane ratings for regular-grade gasoline are an enabler for higher compression ratio, downsizing, turbocharging, downspeeding, and hybridization technologies and that "increasing compression ratios for future SI engines would be the primary response to a significant increase in fuel octane ratings." Furthermore, they state, "higher ethanol content is one available option for increasing the octane ratings of gasoline and would provide additional engine efficiency benefits for part and full load operation," as shown in Figure 17.

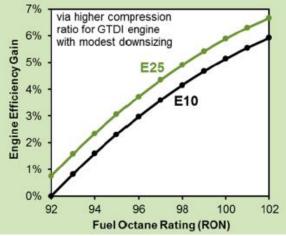


FIGURE 17 ENGINE EFFICIENCY GAINS FROM INCREASING FUEL OCTANE RATING THROUGH ETHANOL CONTENT AND COMPRESSION RATIO INCREASES FOR A GTDI ENGINE WITH MODEST DOWNSIZING (FROM LEONE, 2015)



The biofuels industry would need to take steps to increase the production of ethanol in the US to meet the demand for high octane fuels. Increased production likely would come from both corn starch and cellulosic feedstocks, such as corn stover. Cellulosic biofuels are credited with reducing GHG by at least 60% under the Renewable Fuels Standard (RFS), which would further enhance the lifecycle carbon emissions benefits of a move to ethanol-based high octane fuels. In addition, the gasoline retailing industry would obviously need to ensure the gasoline dispensing equipment is capable of storing and dispensing higher levels of ethanol content in gasoline.

GM and Honda executives said that raising the octane level of pump gasoline in the U.S. is integral to optimizing advanced combustion engines now in development. At the 2016 CAR Management Briefing Seminars Dan Nicholson, VP of Global Propulsion Systems at GM, said, "higher octane fuels are the cheapest CO<sub>2</sub> reduction on a well-to-wheels analysis (SAE International 2016). Fuels and engines must be designed as a total system." Robert Bienenfeld, Assistant VP of Environment and Energy Strategy at American Honda agreed the industry must push for a higher fuel-octane floor in the U.S. prompting positive comments from EPA Director Chris Grundler, noting that the EPA is participating in the U.S. Dept. of Energy's Co-Optima program and has a group working on gasoline octane levels of future fuels.

Chow and coworkers at MIT (Chow, Heywood and Speth 2014) also examined the benefits of a higher octane standard gasoline for the U.S. light-duty vehicle fleet and found "ultimately by redesigning vehicles to take advantage of premium gasoline, fleet fuel consumption and GHG emissions can be reduced by 4.5-6.0% (for 98 RON-100 RON, respectively) over the baseline case, where no additional higher-octane vehicles are introduced."

In a 2017 SAE paper, Darlington (Darlington, et al. 2017) use GHG emissions savings estimates from Leone (Leone, Olin, et al. 2014) for high octane, low carbon fuel (HOLCF) paired with a turbocharged DI engine having it's compression ratio (CR) increased to take advantage of the high octane mid-level ethanol blend fuels.<sup>3</sup> Darlington, 2017 also cite Leone, 2015 and calculate an average benefit level for a 98-RON E25 blend as about 6% for most engines. In terms of vehicle range, Leone, 2014 also found that the 13:1 compression ratio engine gave similar driving range on a 101-RON E30 fuel than the baseline 10:1 engine with regular E10 fuel.

<sup>&</sup>lt;sup>3</sup> The results of Leone, 2014 indicate that 96-RON E20 fuel enables an increase from 10:1 to 11.9:1 CR and 101-RON E30 fuel enables a further CR increase to 13.0:1 with GHG benefits of roughly 5% and 6%, respectively, on the EPA city/highway cycle; however on the more aggressive US06 cycle the benefit level grows slightly for the 96-RON E20 but more substantially to 9% for the 98-RON E30.



## 5.4 Greenhouse Gas Emissions of High-Octane, Mid-Level Ethanol Blends

The DOE (Theiss, et al. 2016) has recently published a summary of its efforts investigating the potential of High Octane Fuel (HOF) with 25-40% ethanol blends. DOE investigators came together from Oak Ridge National Laboratory, National Renewable Energy Laboratory, and Argonne National Laboratory with the objective of providing a quantitative picture of the barriers to adoption of HOF and the highly efficient vehicles it enables, and to quantify the potential environmental and economic benefits of the technology. The results of these studies, considered together, show that HOF mid-level ethanol blends could offer significant benefits for the United States. These benefits include a 5-10% efficiency increase in vehicles designed for increased ethanol content and a miles-per-gallon fuel economy parity with E10.

Furthermore, dedicated HOF vehicles exhibit nearly 15% lower well-to-wheels GHG emissions resulting from increased vehicle efficiency and corn ethanol production and use; future corn stover use shows potential to increase the well-to-wheels (WtW) savings to around 30%, Figure 18. By increasing the percentage of ethanol in the fuel supply, the amount of gasoline consumed decreases, thereby further reducing the nation's dependency on crude oil imports and enhancing U.S. energy security.

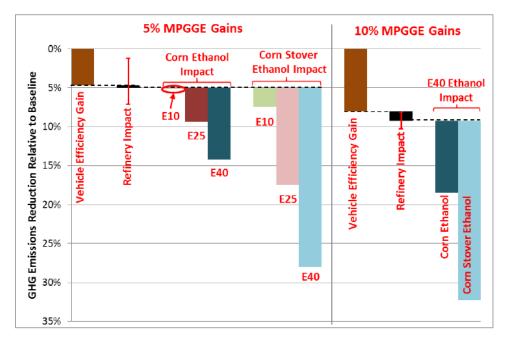


FIGURE 18 WTW GHG EMISSIONS REDUCTIONS IN VEHICLES FUELD BY HOFS WITH DIFFERENT ETHANOL BLENDING LEVELS RELATIVE TO REGULAR GASOLINE (E10) BASELINE VEHICLES (FROM THEISS, 2016)

Kwasniewski et al (Kwasniewski, Blieszner and Nelson 2016) also studied the impact on refinery GHG emissions for 10% and 30% ethanol blends with varying octane ratings. The study found that refinery GHG emissions decline 12% to 27% from a 2017 baseline for the



various 30% ethanol cases due to both the extensive effect of lower crude oil throughput and the generally-overlooked intensive effects of differences in the severity of refining operations.

# 6 ECONOMICS OF HIGH OCTANE FUELS (HOF)

There have been a number of recent studies related to the economics of increasing the octane levels by raising the ethanol content of gasolines sold in the U.S. and also the cost savings produced by HOLCF use in engines with increased compression ratios.

To estimate the cost of a CR increase that is enabled by HOLCF, Darlington, 2017 cite a National Academy of Sciences study (National Academy of Sciences 2015) and average their cost range to get \$100 for improved pistons and rings. The savings in fuel cost resulting from the change to HOLCF was estimated at a net present value of \$132, and note that the incremental technology cost approximately balances out the fuel saving credit, using a net zero cost to the consumer. In exercising the EPA's OMEGA model for the impact of HOLCF with high CR engines, Darlington, 2017 found the cost of meeting the model year 2025 GHG emission standards is reduced on a national basis from \$23.4B to \$16.4B.

Speth and associates at MIT (Speth, et al. 2014) modeled the potential macro-economic effects of transitioning to high-octane (98 RON) gasoline by 2040. They found that if high-octane gasoline in appropriately tuned vehicles accounted for 80% of consumption in 2040, a 3.0-4.4% reduction in total gasoline energy consumption could be achieved. This coincides with a 19-35 metric ton reduction in  $CO_2$  emissions in 2040. The direct national economic benefit of using high-octane fuel is estimated to be \$0.4–6.4 billion in 2040, and rises to \$1.7–8.8 billion if the social cost of avoided carbon emissions is included.

Hirshfeld, 2014 created a model of the refining economics of US gasoline with particular focus on the octane ratings and ethanol content, Figure 19. The model also examined the impacts of these factors on  $CO_2$  emissions and crude oil use.



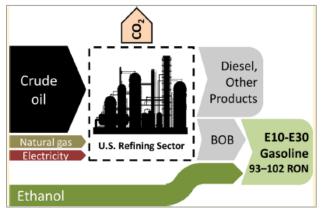


FIGURE 19 MODEL OF US GASOLINE REFINING AND BLENDING WITH ETHANOL (FROM HIRSHFELD, 2014)

Using their linear programming model, Hirshfeld, 2014 examined two ways of increasing the octane of the finished gasoline: by increasing the octane of the petroleum blendstock for oxygenate blending (BOB) and by increasing the volume fraction of ethanol. As shown in Figure 20, increasing the ethanol content of the finished fuel is the lowest-cost means of achieving a higher RON rating. For example, to achieve a 98 RON standard with only 10% ethanol, the additional refining cost is approximately \$0.20/gallon. However, a lower cost approach would be to achieve the 98 RON standard by adding 30% ethanol to the gasoline blendstock to make E30 at an additional refining cost of just \$0.02/gallon—ten times less costly than the E10 scenario. Due to the efficiency increases enabled by higher octane fuels and the displacement of petroleum by ethanol, the study also found that using E30 to achieve a 98 RON standard would result in the reduction of refinery CO<sub>2</sub> emissions by 3-10% and the reduction of crude oil throughput for gasoline refining by 3-8% compared to the case where E10 is used to meet the 98 RON standard.

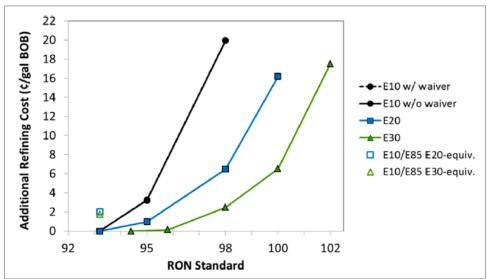


FIGURE 20 ADDITIONAL REFINING COST FOR VARIOUS RON LEVELS AND ETHANOL CONTENTS (FROM HIRSHFELD, 2014)



Relevant to the discussion over the economics of potential future high octane fuels is an analysis by the University of Illinois Department of Agricultural and Consumer Economics (Irwin and Good 2017), which looked at the historical economic value of ethanol in the gasoline blend. The authors state that previous analyses of ethanol's economic value have often adjusted the market value to account for the lower volumetric energy content of ethanol relative to conventional gasoline blendstock for oxygenate blending (CBOB). They suggest that while ethanol generally has had a lower absolute price per gallon on average than CBOB, when adjusted for energy content, ethanol has often been more expensive than CBOB. However, one of the factors that has been neglected has been the value of ethanol as an octane enhancer in gasoline. Ethanol replaces costly aromatic compunds that are used to increase the octane of conventional gasoline made with CBOB. These aromatic octane boosters are sold at a significant price premium, called the "octane premium." An example of these two factors are shown in Figure 21 for the previous 10 year period at the U.S. Gulf.

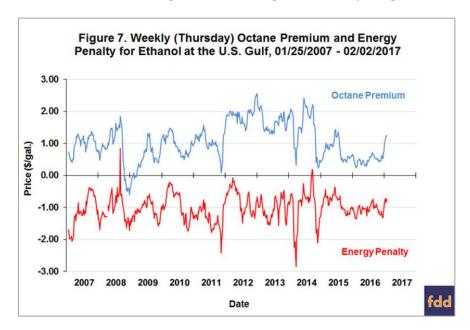


FIGURE 21 WEEKLY OCTANE PREMIUM AND ENERGY PENALTY FOR ETHANOL (FROM IRWIN, 2017)

According to the authors, ethanol's "octane premium" value has typically offset its so-called "energy penalty" over the past decade, as shown in Figure 24.



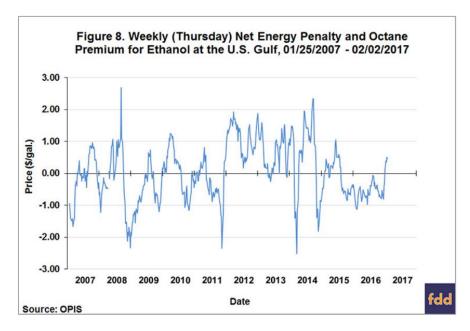


FIGURE 22 NET ENERGY PENALTY AND OCTANE PREMIUM FOR ETHANOL (FROM IRWIN, 2017)

The authors calculated that the fuel ethanol contribution to gasoline provided a net cost reduction of nearly \$7 billion dollars between 2008 and 2016. As this analysis is backward-looking, it does not consider the further value ethanol will have in increasing the octane of the gasoline blend to enable high compression ratio engines, without significant refinery capital investment to increase octane production.

Moriarty (Moriarty, Kass and Theiss 2014) have evaluated the implications on the gasoline distribution network of introducing high octane fuels containing 25% or more ethanol, identifying deployment issues that remain to be resolved. Fuel dispensing equipment is certified by the UL (UL LLC 2009) and currently available for E10, E25 and E85 fuels through UL 87A pathways. E25 equipment is very close in price to E10 equipment, in fact one manufacturer has stopped offering E10 equipment for sale, but there is a significant cost premium for E85 dispensing equipment. In order for service stations to dispense an E30 or E40 gasoline, some work remains to be done to assure that the appropriately validated dispensing equipment is available and installed. Moriarty, 2014 concluded that E25 would be the easiest and least costly of the high octane fuels to be deployed, because of the limitations of the existing dispensing equipment. The majority of underground tanks were judged to be capable of storing ethanol blends up to E85, but there are concerns that many stations would need to add another tank to add a higher ethanol blend without eliminating an existing fuel. Lastly, the authors thought the largest barrier to implementation of mid-level ethanol blends is that service stations are not required to keep records of their equipment, so that many station owners are not aware of the capabilities of their equipment.



A market analysis was initiated by the DOE Bioenergy Technologies Office as part of a collaborative research program and summarized by Theiss, 2016 which developed eight deployment scenarios for vehicles adapted for use of High Octane Fuels. These scenarios were modeled by the Automotive Deployment Options Tool (ADOPT). Modeling results showed that E40 was the most likely blend to be accepted by consumers because of the lower costs for consumers and the large greenhouse gas emissions reductions for the automakers. This prediction contradicts the Moriarty, 2014 study which focused only on infrastructure implications and found that E25 is the most easily adopted blend because of existing dispenser certification levels. The model further predicted that more than 60% of light duty liquid fuel could be an E40 blend by 2035. More work will be needed to determine the most economically and technically viable pathway for increasing the ethanol content of high octane fuels.

## 7 CONCLUSIONS

Modern gasoline engines continue to be developed for ever greater fuel efficiency and performance levels, driven principally by light-duty vehicle standards for greenhouse gas emission and fuel economy. This literature review study found that fuel economy is being improved through the parallel pathways of engine boosting combined with downsizing and increased geometric compression ratio combined with modified inlet valve closing strategies. Both approaches, however, are limited by engine knock. The study also found that another technology that would enable further improvements in engine efficiency is the use of high-octane gasolines blended with ethanol. Gasolines having ethanol in the 15% - 40% range can be blended to increase the anti-knock index (AKI = [RON + MON]/2) thereby enabling engine efficiency improvements.

High octane, mid-level ethanol blends have anti-knock qualities that go beyond it's simple AKI rating, however. Ethanol's high sensitivity (S = RON – MON) and its high heat of vaporization means that engine performance and efficiency can be increased for direct injection (DI) engines more than is indicated by the RON value of the fuel.

The results from the studies reviewed generally support a main conclusion that splash blending ethanol is a highly effective means of raising the octane rating of gasoline and enabling low-cost efficiencies and reduced emissions in modern spark-ignition engines.



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