Fuel/Engine Interactions:
Potential for Emissions and Efficiency Improvement

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Introduction

Although fully-electric and H_2 fuel cell vehicles are now available in the market, internal combustion (IC) engines are expected to make up the bulk of the US vehicle fleet for the foreseeable future. Figure 1 shows projected vehicle sales for the next decade. Note that gasoline-engine powered vehicles are anticipated to dominate new vehicle sales through 2025, and will continue to make up the bulk of the existing vehicle fleet for many years afterwards. Indeed, the reference case scenario of the U.S. Energy Information Agency's 2014 Annual Energy Outlook projects that even by 2040, over 99% of vehicles sold will have internal combustion engines. Within the US, these engines will predominantly use gasoline-like fuels, though we expect that the fraction of renewable fuels will increase considerably over this period.

Although IC engines have seen continuous improvements in efficiency, power-density, and emissions performance over the last 100 years, they are designed to run on currently available fuels. Consequently their efficiency and performance is compromised. In light of their anticipated continued dominance, and potential large upcoming changes in the composition of the fuel supply, examination of the engine efficiency gains that could be enabled by changes in fuel properties is of considerable interest.

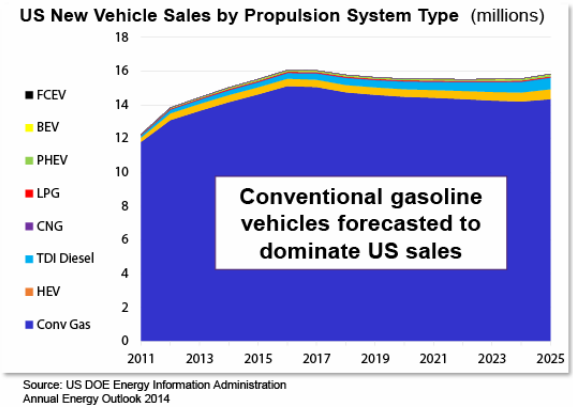

Figure 1: Projected US light-duty vehicles sales through 2025

Properties enabling efficiency gains

<u>Octane rating</u> Commencing with the first engines developed by Nicolaus Otto, performance has been limited by knock, and the knock resistance or autoignition characteristics of the fuel continues to be the fuel property having the greatest impact on engine efficiency. In the US fuel knock resistance is characterized by the research and motor octane numbers, RON and MON, which are measured in a test engine with intake mixture temperatures in the range of ~40° C and ~150° C, respectively (see ASTM test methods D2699 and D2700 for further details). Autoignition in modern engines, operating with intake temperatures closer to those of the RON test, correlate much better with RON than with MON. Nevertheless, MON remains a relevant parameter since the fuel "Sensitivity", defined as RON-MON, has been shown to have a beneficial impact on the knock performance of modern engines.

The potential benefit of increased RON on engine efficiency is typically determined in a two-step process. First, the increase in the octane number needed to increase engine compression ratio is determined, followed by estimation of the efficiency gain enabled by the increased compression ratio. Estimates of the octane number increase needed to increase the engine

compression ratio by one point vary throughout the literature, since it depends on engine technology, geometry, and operating conditions. Recent surveys by academic or research institutions suggest that a RON increase of 4-5 points is needed. In contrast, authors associated with the car manufacturers believe that a RON increase of only 3 points is needed – citing the need to make this determination using consistent design practices. That is, changing the compression ratio is not as simple as making a piston change, but must also involve careful optimization of the in-cylinder flow, mixture formation, and localized heat transfer rates. Likewise, the efficiency gain that can be achieved with a unit increase in compression ratio is not easily determined, as it depends on displacement, speed, load, and the initial compression ratio. An increase in relative efficiency of 1.6% for each unit increase in compression ratio, however, is a conservative value that can be used for estimation. This value accounts for the thermodynamic benefit of an increased expansion ratio as well as the ability to more optimally phase the combustion process when knock resistant fuels are used.

There is an additional multiplicative benefit to the increased efficiency cited above. Increasing the engine efficiency results in higher torque, and thus allows one to use a smaller engine to meet the same torque requirement or to run the engine at a lower speed to meet the same power requirement. “Down-sizing” or “down-speeding’ the engine in turn provides additional benefits associated with reduced mass and/or friction. Consequently, the direct efficiency gain observed with an increase in compression ratio can be multiplied by a factor of 1.3 for naturally aspirated engines, or by 1.1 for turbocharged engines – which have already reaped many of the benefits of downsizing.

Finally, we consider the benefit of fuel Sensitivity on knock resistance. A fuel’s effective knock resistance, at operating conditions between the RON and MON tests, can be expressed as an octane index (OI) which interpolates between RON and MON as shown by the first expression in the equation below:

$$\begin{aligned} OI &= (1-K)*RON + K*MON \\ &= RON - K*(RON - MON) \end{aligned}$$

Modern engines typically have intake conditions “beyond RON,” however, and an octane index that best correlates engine knock performance is found when the interpolative constant *K* takes values less than zero. *K* depends on the pressure and temperature history that the fuel-air mixture experiences, and thus varies over the engine operating map, but an average value of approximately -0.5 seems representative of modern, turbocharged engines. Re-writing the above equation in the second form shows that with negative *K*, fuels with a high sensitivity have higher knock resistance than would be expected from the fuel RON alone.

<u>Fuel distillation characteristics</u> Various properties related to a fuel’s vaporization behavior also impact efficiency. One of the most controversial of these is the heat-of-vaporization (HoV). In modern direct-injection engines, one expects that fuels with a high HoV will impart additional knock resistance due to charge cooling associated with the fuel vaporization processes. Several authors have argued that HoV effects can be quite large in direct-injection engines, and impart an additional knock resistance equivalent to ~5 octane points over port-injected engines with fuels having gasoline-like HoVs. Fuels such as alcohols can have several times the heat of vaporization of gasoline, and have been reported to provide up to 18 additional octane points for a fuel made up of 85% ethanol. More recent studies have tended to downplay this advantage,

however, and indicate that for ethanol fractions below approximately 40% the additional HoV confers little advantage. These studies argue that the impact of HoV is already factored in to the fuel RON. This is a topic that requires significant additional clarification, and hence we do not consider effective octane increases due to HoV in the estimates of potential fuel efficiency gains given below.

Heat of vaporization can impact engine efficiency through avenues other than knock resistance, however. Charge cooling affects heat transfer and pumping work, in addition to introducing "bookkeeping" biases into the calculated thermal efficiency. The latter arises from the fact that HoV figures prominently into the determination of a fuel's heating value, which is used to translate measured fuel consumption into engine thermal efficiency. Because the energy needed to vaporize the fuel is available for "free" in engine applications, a metric more closely approximated by the net chemical energy released would be preferred to perform this translation. Overall, we can assign an increase in thermal efficiency of ~1% for every 250 KJ/kg increment in HoV over gasoline.

Other vaporization related properties also impact efficiency, albeit indirectly. Vapor pressure, T90 (the 90% mass-loss distillation temperature), and HoV all correlate with soot production. Excessive engine soot emissions may force calibration changes or adoption of particulate filters that result in fuel economy degradation. T90 also impacts fuel spray liquid penetration, which can thus affect the amount of downsizing that can be achieved without incurring significant wall-wetting. Wall wetting also impacts preignition, and may thus influence the ability to achieve efficient low-speed, high-load operation.

<u>Flame speed</u> Fuels with high flame speeds impact efficiency by reducing burn time. Reduced burn time at fixed spark timing impacts efficiency by effectively advancing the combustion phasing, allowing for greater work extraction by expansion. By shortening combustion and the time available for autoignition reactions to occur, high flame speed fuels also allow greater spark advance, further increasing engine efficiency. By using fuel blendstocks with high flame speeds, obtained by adding high-flame speed renewables or by tuning refinery processes to create outputs high in olefins, efficiency improvements of ~1% can be expected for every increase in flame speed of 3 cm/s.

Estimated potential efficiency gains

Efficiency gains for two different potential fuel scenarios are shown in Figure 2. The first, baseline, scenario envisions the use of a 15 volume-percent ethanol blend in a petroleum blendstock with a RON of 94 and MON of 86. The resulting blend will have a RON of 100 and MON of 88, or a Sensitivity of 12. In comparison with a current RON 91 fuel with a sensitivity of 8, this allows for an increase in engine efficiency of approximately 7.6% due to improved autoignition resistance alone. Accounting for additional HoV effects, as well as an anticipated increase in flame speed of 3 cm/s, we could expect an overall, fuel-enabled increase in engine efficiency of 9%. The second scenario is

Figure 2: Fuel-enabled efficiency gains achievable for two different fuel scenarios

more aggressive, but still plausible, and demonstrates that fuel-enabled efficiency gains approaching 15% are within reach.

Summary

Combustion engines will remain a mainstay of the light-duty fleet for many years, and within the US SI engines are expected to continue to dominate the light-duty fleet. Although SI engine efficiency has steadily increased, and down-sized boosted concepts are closing the gap between SI and diesel engine efficiencies, there are significant additional engine efficiency gains that can be achieved if fuel properties are tailored appropriately. Fuel autoignition resistance is first among these properties, but the fuel's distillation characteristics and flame speed can also play a significant role.

Two additional points will be made in closing. First, engine designers must be able to count on having tightly controlled fuel properties, with widespread availability, in order to achieve the promised efficiency gains. If engine designs are compromised to enable satisfactory operation over a wide range of fuel properties the potential efficiency benefits will not be achieved. Second, the complete fuel life cycle must be considered in order to ensure that overall energy efficiency and greenhouse gas reduction goals are met. In this respect, producing high-sensitivity fuels may be particularly advantageous, as increasing fuel MON is generally an energy intensive process.