U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

SAND2016-12502R

Co-Optimization of Fuels & Engines

Thrust I Fuel Merit Function

A Tool for Ranking Fuel-Enabled Efficiency Gains When Multiple Fuel Properties Vary Simultaneously

U.S. DEPARTMENT OF ENERGY

Sandia National Laboratories

About the Co-Optimization of Fuels & Engines Project

This is one of a series of reports produced as a result of the Co-Optimization of Fuels & Engines (Co-Optima) project, a Department of Energy (DOE)-sponsored multi-agency project initiated to accelerate the introduction of affordable, scalable, and sustainable biofuels and high-efficiency, low-emission vehicle engines. The simultaneous fuels and vehicles research and development is designed to deliver maximum energy savings, emissions reduction, and on-road performance.

Co-Optima brings together two DOE Office of Energy Efficiency & Renewable Energy (EERE) research offices, nine national laboratories, and numerous industry and academic partners to make improvements to the types of fuels and engines found in most vehicles currently on the road, as well as to develop revolutionary engine technologies for a longer-term, higher-impact series of solutions. This first-of-its-kind project will provide industry with the scientific underpinnings required to move new biofuels and advanced engine systems to market faster while identifying and addressing barriers to commercialization.

In addition to the EERE Vehicle Technologies and Bioenergy Technologies Offices, the Co-Optima project team included representatives from the National Renewable Energy Laboratory and Argonne, Idaho, Lawrence Berkeley, Lawrence Livermore, Los Alamos, Oak Ridge, Pacific Northwest, and Sandia National Laboratories. More detail on the project, as well as the full series of reports, can be found at www.energy.gov/fuel-engine-co-optimization.

Availability

This report is available electronically at no cost from http://www.osti.gov/bridge.

Citation

Miles, Paul. *Thrust I Fuel Merit Function: A Tool for Ranking Fuel-Enabled Efficiency Gains When Multiple Fuel Properties Vary Simultaneously.* (Technical Report) Sandia National Laboratories, 2016.
osti link

Note

Report Contributors and Roles

Lead Author(s)

Lead author

Paul Miles, Sandia National Laboratory

Acknowledgments

This report and the work described were sponsored by the U.S. Department of Energy (DOE) Bioenergy Technologies Office (BETO) and Vehicle Technologies Office (VTO) under the DOE Co-Optimization of Fuels and Engines Initiative. The authors gratefully acknowledge the support and direction of Alicia Lindauer at BETO, Kevin Stork at VTO, and the Co-Optima leadership team.

The following U.S. Department of Energy Office of Energy Efficiency and Renewable Energy (EERE) officials and managers played important roles in establishing the project concept, advancing implementation, and providing ongoing guidance:

Reuben Sarkar, Deputy Assistant Secretary for Transportation

Bioenergy Technologies Office

Jonathan Male, Director

Alicia Lindauer, Technology Manager

Borka Kostova, Technology Manager

Vehicle Technologies Office

Michael Berube, Director

Gurpreet Singh, Program Manager, Advanced Combustion Engines Program

Kevin Stork, Technology Manager, Fuel Technologies and Deployment

Leo Breton, Technology Development Manager

Mike Weismiller, Technology Development Manager

The national laboratory project management team consisted of:

John Farrell (Technical Monitor), National Renewable Energy Laboratory (NREL)

John Holladay, Pacific Northwest National Laboratory (PNNL)

Robert Wagner, Oak Ridge National Laboratory (ORNL)

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Table of Contents

Abbreviations and Acronyms

CO	Carbon monoxide
DI	Direct Injection or Drivability Index
Exx	A gasoline-ethanol blend with xx% ethanol by volume
GPF	Gasoline Particulate Filter
HC	HydroCarbon
HoV	Heat of Vaporization
LFV150	Liquid Fuel Volume remaining at a temperature of 150°C
LSPI	Low Speed Pre-Ignition
MON	Motor Octane Number
OI	Octane Index
PMI	Particulate Matter Index
RON	Research Octane Number
SI	Spark Ignition
Txx	The Temperature at which xx% of a fuel sample is evaporated

1 Thrust I Fuel Merit Function

To assist in making an initial down-selection of promising fuel blendstock candidates, it is useful to define a fuel "Merit Function." This tool is intended to help rank blendstock candidates in a systematic manner when multiple fuel properties are varying simultaneously. Impacts of blendstocks that must necessarily be considered in a ranking process include:

1. the potential for efficiency gains in an engine
2. the impact on criteria emissions
3. vehicle fuel system and after-treatment costs
4. blendstock production scale and economics
5. blendstock life-cycle greenhouse gas emissions
6. blendstock infrastructure compatibility
7. customer acceptance criteria

Here we focus mainly on the first criterion, and attempt to define "merit" based on the blended fuel's impact on engine efficiency. Coupled with appropriate vehicle assumptions and modeling in a framework such as *Autonomie*, this "merit function" allows fuel economy gains to be estimated based on fuel properties. Incorporated in this function is a factor related to the anticipated volume of the blendstock that can be produced or, alternatively, the fraction of the blendstock that can be tolerated in the base fuel.

Some fuel properties may also impact initial vehicle cost—primarily due to higher after-treatment or fuel system costs. Often the additional costs associated with a specific property are unknown. However, where a reasonable cost estimate exists we cite it to provide some assistance to the ASSERT and Market Transformation teams as they work towards defining the overall costs/benefits of a given fuel blendstock. We anticipate that these overall costs will couple fuel economy, vehicle cost, fuel production cost, and other costs associated with infrastructure development, climate and health impacts, and other societal issues. We also hope that the original equipment manufacturers can provide some additional cost estimates as the fuel ranking process matures.

In addition to the considerations listed above, a fuel must possess a number of other qualities in order to be considered practical. For example, it should be soluble in hydrocarbon blendstocks, it should not be a known carcinogen or teratogen, and it should not result in blended fuel properties that are inconsistent with current specifications for distillation metrics, vapor pressure, corrosivity, flashpoint, etc. These additional considerations have been described in greater detail in the LGGF FY16Q1 Milestone report.

The merit function described here is applicable only to "Thrust I" fuel blendstocks targeted at stoichiometric, spark-ignition engines operating in conventional flame propagation combustion modes. For some of the fuel properties considered the formulation of the merit function is currently based on very incomplete information—particularly when the interactions between efficiency and after-treatment devices or pre-ignition phenomena must be considered. Clarifying and quantifying these interactions is one of the central outcomes of the research to be performed by the Advanced Engine Development and Fuel Properties teams. Accordingly, we view the formulation presented here as a first approximation that will need to be refined considerably as the state of our knowledge progresses.

1.1 Brake Fuel Efficiency Merit Function Basis

The merit of a blendstock is assessed by the efficiency gain achieved when blended with a baseline fuel representative of a current "regular" gasoline grade. This grade is assumed to have a Research Octane Number (RON) of 91 and a Motor Octane Number (MON) of 83, giving a Sensitivity (S=RON-MON) of 8 and anti-knock index (AKI) of 87. We also assume a baseline fuel ethanol content of 10 vol%, yielding a HoV of 415 kJ/kg, a flame speed of 46 cm/s, a lower heating value (LHV) of 42 MJ/kg, and a particulate matter index (PMI) of 1.4. The ethanol mole fraction is approximately 0.21 when calculated with a liquid molar volume ratio of 0.42 (see Anderson et al. 2012). Such a fuel could be produced by blending ethanol with a petroleum-based Blendstock for Oxygenate Blending (BOB) with a RON = 84, a MON=79, a HoV=350 kJ/kg, a flame speed of 44 cm/s, a LHV of 43.8 MJ/kg, and a PMI of 1.5.

The merit function is written as a linear combination of the blended fuel properties that are expected to exert a significant impact on efficiency. Blending models that allow the prediction of mixture properties are still being developed; accordingly, we propose adopting a simple linear model based on the fuel mixture blendstock properties P_i and the mole fraction of each blendstock χ_i:

$$P_{mix} = \sum_i \chi_i P_i \tag{1}$$

Much of the non-linearity in mixture properties, such as mixture RON, is removed when the mixture properties are computed based on mole fraction rather than mass fraction or volume fraction. We anticipate that with this formulation the mole fraction of the blendstock can reflect realistic estimates of potential production volume developed by the ASSERT team.

Our initial merit function is written as:

$$\begin{aligned} Merit = {} & \frac{(RON_{mix}-91)}{1.6} - K\frac{(S_{mix}-8)}{1.6} + \frac{0.01[ON/kJ/kg](HoV_{mix}-415[kJ/kg])}{1.6} \\ & + \frac{(HoV_{mix}-415[kJ/kg])}{130} + \frac{(S_{L\,mix}-46[cm/s])}{3} \\ & - LFV_{150} - H\left(PMI-2.0\right)\left[0.67+0.5\left(PMI-2.0\right)\right] \end{aligned} \tag{2}$$

$H(x)$ represents the Heaviside function. A brief discussion of each of the terms follows.

1.1.1 RON & Sensitivity S

Fuel octane is a measure of its knock resistance. Here we follow Kalghatgi (2001) and use the Octane Index (OI) to characterize a fuel's effective octane rating:

$$OI = RON - KS \tag{3}$$

where S is the fuel sensitivity and K is an engine-dependent constant that depends on design parameters and operating conditions. A representative K value for down-sized boosted engines is -0.5; however, this is left as a free parameter in the merit function. Increasing OI allows engine compression ratio to be raised, leading to a higher thermodynamic efficiency. However, even at a fixed compression ratio, higher OI allows engine operation at mid-to-high loads with a greater knock-limited spark advance (KLSA), also resulting in higher efficiency.

Determining the impact of OI on engine efficiency is not straightforward, as it encompasses both engine design parameters as well as the engine's operating profile within the speed/load map. Here we follow the two-step approach of Chow et al. (2014) and Leone et al. (2015), among others. First, we assume that an increase in OI of three points will allow an increase in engine compression ratio of 1, which in turn results in an average increase in efficiency of about 1.6%. Due to the increased efficiency, as well as improved knock-limited performance, the engine will produce higher torque and can be downsized—resulting in additional efficiency improvements. This efficiency boot-strapping effect of downsizing is expected to differ between naturally aspirated and boosted engines, but using an additional efficiency multiplier of 1.2 represents an average expected gain. Consequently, an increase in OI of 3 leads to an expected increase in efficiency of 1.9%, or equivalently an increase in OI of 1.6 leads to an efficiency increase of 1%. Normalization of the terms in the merit function related to OI (RON and S) by the factor 1.6 thus makes their value correspond to the expected percentage increase in efficiency.

Note that this efficiency increase is an expected "average" over the speed-load map. When coupled with *Autonomie*-like modeling to deduce the associated fuel economy improvement, previous work has applied the efficiency increase uniformly over the engine speed-load map (Chow et al. 2014).

1.1.2 Heat of Vaporization (HoV)

Knock can be mitigated both through the inherent chemical autoignition resistance of a fuel represented by the octane index, or by charge cooling. For direct-injection engines, the in-cylinder vaporization process reduces the charge temperature and can thus potentially provide improved efficiency through knock mitigation—Leone et al. (2015) provides additional background and a recent review.

There is a lack of consensus in the literature regarding the magnitude of the impact of charge cooling from fuel vaporization. A comprehensive, multi-cylinder engine study has indicated that, for ethanol fractions less than 30%, there is a negligible impact of HoV on KLSA and brake thermal efficiency at low-to-moderate loads when RON and MON are held constant (Leone et al. 2014). In contrast, Kasseris and Heywood (2012) report that increased HoV increases the effective octane rating at a rate of about 0.15 ON/ethOH v%, and that the rate of increase is approximately linear in ethOH fraction. Still other studies provide evidence that the impact of HoV is at least partially included in the RON test (Stein et al. 2012; Foong et al. 2013), and may not need to be accounted for separately. The latter study indicates that for ethanol fractions below about 40%, increasing HoV increases a fuel's effective octane rating at a rate of only about 40% of the rate of high ethanol blends. The issue is further complicated by the expectation that the fuel sensitivity impacts the effectiveness of vaporization cooling. Until further clarification is obtained, we adopt the position that a fuel's effective OI is impacted only modestly by HoV, and increases at a rate of about 0.01 ON / (kJ/kg). This is equivalent to 0.06 ON/ethOH v% (*cf* 0.16 ON/ethOH v% adopted in Leone et al. (2015) for blends with ethanol fractions greater than 40%).

Heat of vaporization also impacts engine efficiency through other mechanisms. Here we rely largely on the analysis in Jung et al. (2013), which found that vaporization cooling increased the thermal efficiency of a boosted, DI engine by about 4.2% between E0 and E85 or 1% for an increase in HoV of ~130 kJ/kg. This increase was due to reduced HC/CO emissions (~22%), increased pumping work (~-8%), the HoV/LHV ratio[1] (~50%), and the balance is due primarily to reduced heat transfer. The estimate is likely conservative due to the relatively large displacement of the test engine compared to an expected downsized engine displacement.

Although we have limited our considerations to how HoV impacts engine efficiency, it can also have other important impacts on engine operation—such as cold-start behavior.

1.1.3 Flame Speed

There are few studies that directly link fuel flame speed to increased engine efficiency or load. High flame speed benefits part-load operation by decreasing burn duration, which also mitigates knock at high load. Recent work in a highly boosted, downsized DI engine has shown a 1-2% increase in BMEP at fixed spark timing and fueling (Remmert et al. 2014) for fuels formulated to have higher flame speeds. However, the flame speeds were not reported and quantification of the impact of S_L on load or efficiency is not possible. Earlier (Farrell et al. 2003) work clearly showed that cycle-averaged fuel consumption in vehicles with lean-burn, stratified DI engines can be improved by high S_L (potentially high olefin), low aromatic fuels. At high load, engine testing showed high aromatic content appeared to be beneficial. The vehicle tests indicated that the relative thermal efficiency increased by about 1% for every 2-4 cm/s increase in flame speed, depending on the olefin/aromatic content of the fuel. Although these results may not be directly applicable to homogeneous SI engines, in the absence of additional data we adopt them as a first estimate.

1.1.4 Distillation Characteristics

The distillation characteristics of a fuel can impact vehicle fuel economy through multiple mechanisms, all of which are difficult to quantify. For example, fuels with a low Driveability Index (a function of the T10, T50, T90 distillation temperatures) may exhibit greater stability and tolerate greater combustion timing retard during cold starts, thereby shortening the catalyst warm-up phase and decreasing fuel consumption. Distillation characteristics also impact mixture formation, potentially affecting both knock propensity and soot formation—though the impact can be mitigated in the design process through engine-fuel co-optimization. Here we consider only the impact of distillation characteristics on the propensity for low speed pre-ignition (LSPI), which will decrease fuel economy by requiring avoidance of fuel-efficient low-speed, high load regions in the engine operating map.

Recent studies have indicated that cylinder wall-wetting that leads to detachment of fuel-oil droplets from the cylinder wall leads to increased LSPI frequency. A fuel's distillation

[1] The HoV/LHV ratio enters in due to the fact that the fuel HoV detracts from the measured LHV, but is energy that is available "for free" in an engine application.

characteristics impact the vaporization times and locations of liquid phase fuel, and fuels with low volatility are expected to increase wall-wetting and hence LSPI. In a recent (yet unpublished) study that varied fuel distillation characteristics above ~100°C, fuel volatility clearly correlated strongly with LSPI frequency. All of the fuels fell within US and European volatility specifications. The strongest correlation obtained was with the liquid fuel volume remaining at a temperature of 150°C (the approximate liner temperature), which is denoted here LFV_{150}.

To express this as an equivalent fuel economy penalty, we assume that the regions of the speed/load map avoided due to LSPI correspond to speeds below 2000 rpm and loads above 8 bar. Unpublished data obtained from a 2L turbocharged engine indicate that during the US06 cycle 1.3% of the fueled engine cycles fall into this load/speed range, corresponding to approximately 2% of the fuel consumed during the cycle. We assume that the brake thermal efficiency drops by 10%, from 0.36 to 0.33 (fuel consumption increases from 250 to 275 [g/kW-hr]), when the LSPI region is avoided, and that the fraction of time spent avoiding the LSPI region is proportional to LFV_{150}, up to a maximum of 20%:

$$\Delta\eta = -10[\%] * 0.02 * \frac{LFV_{150}}{0.20} = -LFV_{150}[\%]$$

Thus, while the Decision Tree classifies all fuel blendstocks with a boiling point less than 190°C as gasoline like, the merit function penalizes components with a boiling point greater than 150°C.

1.1.5 Particulate Matter Index (PMI)

Although additional work is required to clarify its applicability, the PMI of a fuel has been shown to correlate with particulate mass emissions from PFI engines as well as DI engines (Aikawa et al. 2010; Sobotowski et al. 2015). Depending on the drive cycle, particulate mass can increase several times over for a unit increase in PMI. Likewise, particulate number emissions have been shown to increase with PMI (Aikawa et al. 2010). As a starting point, we assume that mass emissions increase three-fold for every unit increase in PMI.

The increased particulate emissions can impact both engine efficiency and vehicle cost if they necessitate the addition of a gasoline particulate filter (GPF). Although addition of a GPF will degrade fuel economy due to both increased pumping losses and increased potential for knock, recent studies indicate that the impact is minor (Mamakos 2011; Chan et al. 2013; Kern et al. 2014; Mamakos et al. 2013). Guided by the analysis in Mamakos et al. (2013), we assume that over the vehicle lifetime increased backpressure degrades the fuel economy by 0.5% if a particulate filter is required—which we assume corresponds to a PMI > 2.0. Added to this is a 0.17% degradation due to filter regeneration. We also assume that the regeneration frequency is proportional to the particulate mass emissions, tripling for every unit increase in PMI and incurring an additional efficiency penalty of 0.5% for every unit of PMI above 2.0.

Incorporating a GPF will also increase the initial cost of the vehicle, which will depend strongly on vehicle size. Again following Mamakos et al. (2013), we assume a typical GPF cost of ~$200 (160 €). Interestingly, accounting for societal benefits and costs as well, Mamakos et al. (2013) suggest that the net benefit to society of adding a GPF could be negative.

References

Anderson, James E., Thomas G. Leone, Michael H. Shelby, Timothy J. Wallington, Jeffrey J. Bizub, Michael Foster, Michael G. Lynskey, and Dusan Polovina. 2012. "Octane Numbers of Ethanol-Gasoline Blends: Measurements and Novel Estimation Method from Molar Composition," SAE technical paper 2012-01-1274.

Aikawa, K., T. Sakurai, and J.J. Jetter. 2010. "Development of a Predictive Model for Gasoline Vehicle Particulate Matter Emissions." *SAE International Journal of Fuels and Lubricants* 3 (2): 610-622.

Chan, T.W., Eric Meloche, Joseph Kubsh, and Greg Rideout. 2013. "Impact of Ambient Temperature on Gaseous and Particle Emissions from a Direct Injection Gasoline Vehicle and its Implications on Particle Filtration." *SAE International Journal of Fuels and Lubricants* 6 (2): 350-371.

Chow, Eric W., John B. Heywood, and Raymond L. Speth. 2014. "Benefits of a Higher Octane Standard Gasoline for the U.S. Light-Duty Vehicle Fleet," SAE technical paper 2014-01-1961.

Farrell, J.T., W. Weissman, R. J. Johnston, J. Nishimura, T. Ueda, and Y. Iwashita. 2003. "Fuel Effects on SIDI Efficiency and Emissions," SAE technical paper 2003-01-3186.

Foong, Tien Mun, Kai J. Morganti, Michael J. Brear, Gabriel da Silva, Yi Yang, and Frederick L. Dryer. 2013. "The Effect of Charge Cooling on the RON of Ethanol/Gasoline Blends." *SAE International Journal of Fuels and Lubricants* 6 (1): 34-43.

Jung, Hosuk H., Michael H. Shelby, Charles E. Newman, and Robert A. Stein. 2013. "Effect of Ethanol on Part Load Thermal Efficiency and CO2 Emissions of SI Engines." *SAE International Journal of Engines* 6 (1): 456-469.

Kalghatgi, G.T. 2001. "Fuel Anti-Knock Quality - Part I. Engine Studies," SAE technical paper 2001-01-3584.

Kasseris, E. and J.B. Heywood. 2012. "Charge Cooling Effects on Knock Limits in SI DI Engines Using Gasoline/Ethanol Blends: Part 2-Effective Octane Numbers." *SAE International Journal of Fuels and Lubricants* 5 (2): 844-854.

Kern, B., Stephanie Spiess, and Joerg Michael Richter. 2014. "Comprehensive Gasoline Exhaust Gas Aftertreatment, an Effective Measure to Minimize the Contribution of Modern Direct Injection Engines to Fine Dust and Soot Emissions?," SAE technical paper 2014-01-1513.

Leone, Thomas G., James E. Anderson, Richard S. Davis, Asim Iqbal, Ronald A. Reese II, Michael H. Shelby, and William M. Studzinski. 2015. "The Effect of Compression Ratio, Fuel Octane Rating, and Ethanol Content on Spark-Ignition Engine Efficiency." *Environmental Science & Technology* 49 (18): 10778-10789.

Leone, Thomas G., Edward D. Olin, James E. Anderson , Hosuk H. Jung , Michael H. Shelby, and Robert A. Stein. 2014. "Effects of Fuel Octane Rating and Ethanol Content on Knock, Fuel Economy, and CO2 for a Turbocharged DI Engine." *SAE International Journal of Fuels and Lubricants* 7 (1): 9-28.

Mamakos, Athanasio, 2011. *Feasibility of Introducing Particulate Filters on Gasoline Direct Injection Vehicles.* Ispra, Italy: European Commission Joint Research Center – Institute for Energy and Transport.

Mamakos, Athanasio, Nikolaus Steiningerb, Giorgio Martinia, Panagiota Dilaraa, and Yannis Drossinosa. 2013. "Cost effectiveness of particulate filter installation on Direct Injection Gasoline vehicles." *Atmospheric Environment* 77: 16-23.

Remmert, S., S. Campbell, et al. 2014. "Fuel Effects in a Downsized, Highly Boosted Direct Injection Spark Ignition Engine," *23rd Aachen Colloquium on Automobile and Engine Technology*, 807-828. Aachen, Germany: 23rd Aachen Colloquium on Automobile and Engine Technology.

Sobotowski, Rafal A., Aron D. Butler, and Zuimdie Guerra. 2015. "A Pilot Study of Fuel Impacts on PM Emissions from Light-Duty Gasoline Vehicles." *SAE International Journal of Fuels and Lubricants* 8 (1): 214-233.

Stein, Robert A., Dusan Polovina, Kevin Roth , Michael Foster, Michael Lynskey, Todd Whiting, James E. Anderson, Michael H. Shelby, Thomas G. Leone, and Steven VanderGriend. 2012. "Effect of Heat of Vaporization, Chemical Octane, and Sensitivity on Knock Limit for Ethanol - Gasoline Blends." *SAE International Journal of Fuels and Lubricants* 5 (2): 823-843.

U.S. DEPARTMENT OF
ENERGY
Energy Efficiency &
Renewable Energy

Prepared by the National Renewable Energy Laboratory and Sandia National Laboratories for the U.S. Department of Energy.
DOE/GO-xxxxxx-xxxx • December 2016