U.S. DEPARTMENT OF ENERGY
Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Co-Optimization of Fuels & Engines

A Transportation Future with Science in the Driver’s Seat

Mapping a Viable Route Forward for Affordable, Efficient, and Clean Fuels and Engines

March 2020

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About the Co-Optimization of Fuels and Engines Initiative

The Co-Optimization of Fuels & Engines (Co-Optima) initiative, a U.S. Department of Energy (DOE) sponsored effort focuses on the simultaneous investigation of advanced engine technologies and enabling fuel properties. This first-of-its-kind effort is designed to provide American industry with the scientific underpinnings needed to maximize vehicle performance and efficiency, leverage domestic fuel resources, and reduce lifecycle emissions. Co-Optima brings together the Office of Energy Efficiency and Renewable Energy's (EERE) Vehicle Technologies and Bioenergy Technologies Offices, nine national laboratories, and multiple university and industry partners. Learn more at www.energy.gov/fuel-engine-co-optimization.

Availability

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

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Note

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Acknowledgments

This research was conducted as part of the Co-Optimization of Fuels & Engines (Co-Optima) project sponsored by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), Bioenergy Technologies and Vehicle Technologies Offices. Co-Optima is a collaborative project of multiple national laboratories and universities initiated to simultaneously accelerate the introduction of affordable, scalable, and sustainable biofuels and high-efficiency, low-emission vehicle engines.

The partnering national laboratories include Argonne National Laboratory, Idaho National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Renewable Energy Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, and Sandia National Laboratories. The following EERE officials and managers played important roles in establishing the project concept, advancing implementation, and providing ongoing guidance.

DOE Office of Energy Efficiency and Renewable Energy

- Michael Berube, Acting Deputy Assistant Secretary for Transportation

Bioenergy Technologies Office

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- Alicia Lindauer, Technology Manager

Vehicle Technologies Office

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- Robert L. McCormick, National Renewable Energy Laboratory (NREL)

Background and Context

In 2017, for the first time since the 1970s, U.S. cars and trucks emitted more carbon dioxide (CO_2) than power plants.[1] While the power generation sector has realized significant CO_2 reductions in recent years, achieving the same from transportation has proven to be more vexing. More than 90% of the gasoline and diesel sold in the United States comes from petroleum, reflecting beneficial attributes such as high energy density, relatively low cost, mature production facilities, and ubiquitous refueling infrastructure. There still remain significant R&D and infrastructure challenges that must be addressed before lower carbon-intensity alternatives can be competitive at the retail station.

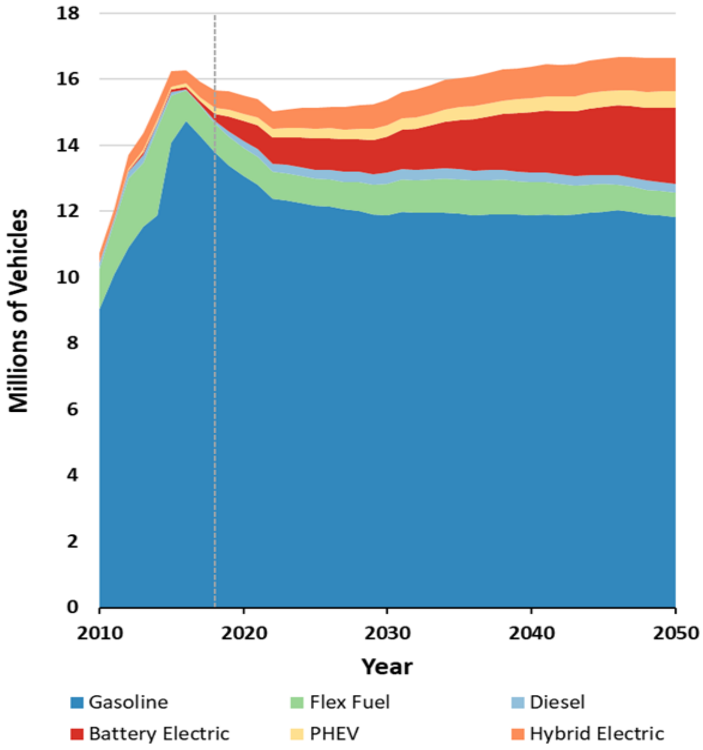

Figure 1. Projections of light-duty vehicles by technology class through 2050[3]

Electric vehicles (EVs) represent an attractive option for some consumers and EV sales have shown significant growth over the past several years, reflecting year-on-year battery cost reductions and expanded access to vehicle charging opportunities. However, EVs make up less than 1% of vehicles on American roads today[2] and even under aggressive growth scenarios, internal combustion engines (ICEs) will dominate new vehicle sales for decades[3] as shown in Figure 1. Consequently, ICE technical solutions are desired that can help minimize lifecycle CO_2 emissions while maintaining affordable powertrain options for U.S. consumers.

There have been numerous discussions and discourse on the options available related to new fuels and engines and it is timely to raise the question: what does the science say about what new fuels and engines should look like?

For the past four years, the U.S. Department of Energy (DOE) has been funding the Co-Optimization of Fuels & Engines (Co-Optima) initiative, focused on identifying fuel properties and engine parameters that impact engine efficiency with the goal of accelerating the commercial

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[1] U.S. Energy Information Administration. "Power Sector Carbon Dioxide Emissions Fall Below Transportation Sector Emissions." January 19, 2017. https://www.eia.gov/todayinenergy/detail.php?id=29612.
[2] N. Boomey. "Americans More Likely to Buy Electric Cars, AAA Study Finds." *USA Today*. May 8, 2018.
[3] U.S. Energy Information Administration. Annual Energy Outlook 2019. https://www.eia.gov/outlooks/aeo/.

introduction of new fuel options that are scalable, sustainable, affordable, and compatible with existing vehicle and retail/distribution infrastructure. The Co-Optima initiative aligns the diverse expertise, world-leading science, and one-of-a-kind science facilities of the national laboratories and universities with significant engagement with industry and government stakeholders. Results are now available that will inform the debate surrounding which fuel/engine options should be considered for the United States in the future.

Scope of Effort

The Co-Optima initiative brings together nine national laboratories and more than 20 university and industry partners to identify the benefits that can be achieved through simultaneous improvements to fuel properties and engine operation. Key goals of the initiative for passenger vehicles include identifying pathways to a minimum 10% increase in fuel economy relative to an expected 2030 baseline (which represents a 35% increase over a 2015 baseline),[4] saving U.S. consumers \$20 to \$30 billion each year through improved vehicle fuel efficiency, diversifying the supply of domestically sourced fuel, and significantly decreasing greenhouse gas emissions from transportation. Although not limited to bio-based fuels, pathways that utilize domestic biomass resources including perennial energy crops, forestry and agricultural residues, or other waste resources can offer even greater reductions and provide long-term sustainable options.

Co-Optima research builds upon and leverages current industry megatrends. U.S. automakers are increasingly replacing conventional ("naturally aspirated") spark-ignition (SI) engines with smaller engines paired with a turbocharger, which are capable of delivering the same power output with improved emissions and fuel economy. A key challenge to realizing the maximum efficiency potential of these turbocharged (or "boosted") SI engines is mitigating engine knock—spontaneous ignition of the unburned fuel/air mixture that can be very damaging to engines.

Co-Optima research to date has been focused on identifying the fuel properties and engine parameters that mitigate knock and thus maximize boosted SI efficiency, emissions, and performance. While Co-Optima is also addressing co-optimization

The Co-Optima team operates according to two central hypotheses:

- **Central Engine Hypothesis***:* There are engine architectures and combustion strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range.
- **Central Fuels Hypothesis***:* If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance.

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[4] U.S. Department of Energy, Office of Energy Efficiency & Renewable Energy, Vehicle Technologies Office. "Advanced Combustion Engines and Fuels 2018 Annual Progress Report." https://www.energy.gov/eere/vehicles/downloads/advanced-combustion-engines-and-fuels-fy2018-annual-progress-report-0.

of advanced compression-ignition combustion approaches, this discussion is limited to boosted SI engines.

For background purposes, gasoline sold at the retail pump is marketed as regular, mid-grade, or premium based on its "pump octane" or anti-knock index (AKI). AKI is the average of two numbers: Research Octane Number (RON) and Motor Octane Number (MON). Together, they make up the numerator of the familiar equation on the pump: (R+M)/2. Both RON and MON are fuel performance metrics established in the 1930s to measure the ability of a fuel to mitigate engine knock under different operating conditions. It is well established that RON is a more relevant metric for assessing anti-knock performance in modern boosted SI engines,[5] though MON is still useful for some engine operating conditions (e.g., aggressive, high-load driving).

Co-Optima research is framed around three interrelated questions:

- What fuels do engines want?
- What fuels should we make?
- What is practical in the real world?

What Fuels Do Engines Want?

If an engine could operate on any possible fuel, what properties would this ideal fuel have so as to maximize efficiency and minimize emissions? Today's engines have been designed to work well with market fuels, but the ultimate efficiency and emissions performance is constrained by their properties. This constraint is even more of an issue with advanced engine designs capable of approaching the theoretical thermodynamic maximum performance, which will require dramatically different fuel properties.

Over the course of three years, Co-Optima researchers performed a number of sophisticated engine experiments focused on developing a comprehensive understanding of the relationship between fuel properties and boosted SI engine parameters (e.g., compression ratio, extent of downsizing, etc.). Central to this effort was development of an engine efficiency "merit function," which is a numerical equation that quantifies the relationship between fuel properties and boosted SI engine efficiency in co-optimized engines.[6] The merit function (shown schematically in Figure 2) quantifies the impact of six fuel properties—RON, octane sensitivity (S), heat of vaporization (HOV), flame speed, particulate matter index (PMI), and catalyst light-off-temperature. Of the fuel properties investigated, these six were found to have the most impact on engine efficiency and emissions. The merit function represents the most detailed correlation developed to date relating fuel properties and engine efficiency, and provides new detailed fundamental understanding of how fuel properties can enable highly efficient boosted SI operation. Because the merit function estimates the percent change in engine efficiency based on changes to fuel properties, it is a much better gauge to assess impacts of fuel changes than

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[5] Wang, Z., H. Liu, and R.D. Reitz. "Knocking Combustion in Spark-Ignition Engines." *Prog Energy Combust Sci* 61:78-112, 2017 http://dx.doi.org/10.1016/j.pecs.2017.03.004.

[6] U.S. Department of Energy Office of Scientific and Technical Information. "Efficiency Merit Function for Spark-Ignition Engines; Revisions and Improvements Based on FY16-17 Research." August 2, 2018. doi:10.2172/1463450.

common metrics such as AKI, which do not relate directly to engine efficiency. The algebraic form of the merit function allows identification of how key fuel properties can be changed and/or traded off to achieve specific efficiency benefits (e.g., how a decrease in RON can be offset by increasing S.)

Co-Optima research has also contributed new fundamental understanding of how in-cylinder temperature, pressure, mixture composition (e.g., dilution), mixture preparation (e.g., direct injection), and fuel kinetics impact knock and, thus, engine efficiency. New insights have also been gained on how fuel properties (in particular, HOV) interact with fuel composition (e.g., high-boiling aromatics) and engine parameters (e.g., fuel injection timing) to produce increased particulate matter (PM). These studies have helped resolve long-standing disputes in the community of how high-HOV fuels—in particular, E10 (gasoline containing 10% ethanol) and mid-level ethanol blends—impact PM formation, and identified strategies for minimizing increased PM formation.

$$\text{Merit} = \overset{\text{RON}}{\boxed{\alpha \bullet f(\text{RON})}} + \overset{\text{Octane Sensitivity}}{\boxed{\beta \bullet f(K, S)}} + \overset{\text{Heat of Vaporization}}{\boxed{\gamma \bullet f(\text{HOV})}}$$

$$+ \underset{\text{Flame Speed}}{\boxed{\varepsilon \bullet f(S_L)}} + \underset{\text{PM Emissions}}{\boxed{\zeta \bullet f(\text{PMI})}} + \underset{\text{Catalyst Light-off Temp (cold start)}}{\boxed{\eta \bullet f(T_{c,90,conv})}}$$

Figure 2. The engine efficiency "merit function" is a numerical relationship that was developed to quantify the relationship between fuel properties and boosted SI engine efficiency in co-optimized engines.

While the six fuel properties included in the merit function all impact engine efficiency, three of these—RON, S, and HOV—are the fuel properties with the greatest impact on boosted SI engine efficiency and consideration of all three—not just RON as proposed by automakers—should factor into considerations of how regular gasoline should change.

What Fuels Should We Make?

With the knowledge that RON, S, and HOV are key properties for advanced boosted engines, we turn to the question of how to blend fuels that provide these properties most cost-effectively. Petroleum refiners have known for decades how to blend hydrocarbons to meet desired fuel properties. However, at the outset of the Co-Optima initiative, the state of understanding for oxygenated hydrocarbons, which can be readily produced from both biomass and fossil resources, was much less developed. Consequently, we focused on bridging the understanding gap between hydrocarbons and oxygenates.

Our evaluation process involved a screening approach that allowed us to efficiently identify blendstocks from diverse chemical families that have the greatest potential to increase boosted SI efficiency, as well as key barriers to their near-term commercialization when sourced from biomass. The results of our screening process identified 10 fuel blendstocks from four chemical families (see Figure 3) that impart the desired properties to a petroleum base fuel.[7] The 10 blendstocks include a variety of alcohols, an olefin, a furan mixture, and a ketone, with the alcohols and olefin exhibiting the fewest barriers to commercial adoption. Of these 10 blendstocks, six were assessed to have the fewest significant practical barriers to adoption which include alcohols and an olefin (alkene): di-isobutylene, ethanol, a fusel alcohol blend, isobutanol, n-propanol, and isopropanol. Several of these blendstocks are relatively new and/or underexplored by the fuels community and represent options that fuel producers and blenders can consider as candidates for inclusion in future fuels.

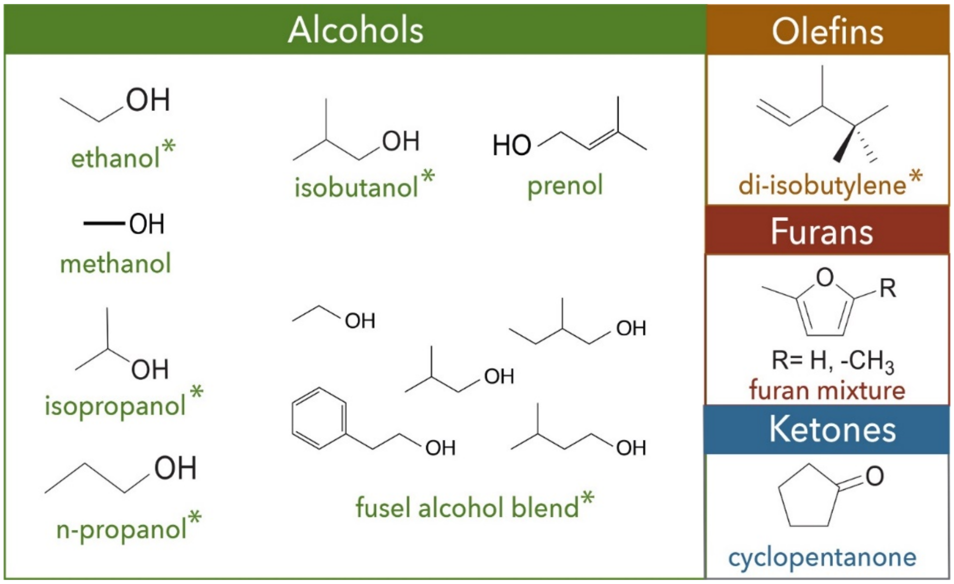

Figure 3. Results of our screening process identified ten blendstocks from four chemical families that impart the desired properties to a petroleum base fuel and have the fewest barriers to commercial introduction. The six blendstocks with asterisks denote those with the fewest commercial barriers.

The Co-Optima blendstock study represents the most comprehensive and consistent comparison of boosted SI fuel blendstocks available in the scientific literature. Just as important as the blendstock list are the fundamental insights and understanding generated, including the development of structure-property relationships that represent the most comprehensive relationship available in the technical literature linking molecular structure to ignition metrics (RON, MON, S), particulate matter formation, thermophysical properties (e.g., Reid vapor pressure, viscosity, surface tension), and HOV. These relationships provide the fundamental understanding required to identify new blendstocks having desirable boosted SI properties.

Collectively, the Co-Optima blendstock identification efforts provide foundational tools, data, and understanding to aid future blendstock and fuel development efforts as biomass conversion methods and engine technologies continue to evolve.

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[7] Gaspar, D.J., B.H. West, D. Ruddy, T.J. Wilke, E. Polikarpov, T.L. Alleman, A. George, et al. "Top Ten Blendstocks Derived from Biomass for Turbocharged Spark Ignition Engines: Bio-blendstocks with Potential for Highest Engine Efficiency." September 2019. doi:10.2172/1567705.

What Will Work in the Real World?

Co-Optima's goal of accelerating the introduction of new fuels and vehicles drove a rigorous screening process to identify promising boosted SI blendstocks for "showstopper" attributes or performance characteristics that constitute significant barriers to commercialization. This includes compatibility of candidate blendstocks with elastomers, plastics, and metals to assess compatibility with vehicles and infrastructure. These studies have indicated that some blendstocks that achieve high engine efficiency merit function scores are fully compatible with current fuel distribution, retailing, and vehicle infrastructure. However, others have deleterious interactions that likely represent significant barriers to commercial use. We have also assessed impacts on key emissions formation/control processes, such as PM formation and catalyst light-off, and identified that many oxygenates provide lower catalyst light-off temperatures than hydrocarbons, providing potential efficiency benefits. We have conducted preliminary screening for low-speed preignition (LSPI), which can result in super-knock, and identified candidates with increased LSPI propensity and thus potential barriers to use in high-efficiency engines. The result of these screening assessments was the identification of the six blendstocks (denoted with an asterisk in Figure 3) that have the fewest barriers to commercial introduction and therefore represent the blendstocks with the greatest potential for near-term impact.

Co-Optima researchers have shown that all the high-performing boosted SI blendstocks can be produced from various resources, including conventional petroleum, natural gas, and renewable domestic feedstocks that offer significantly lower lifecycle greenhouse gas emissions and other benefits, such as increased domestic fuel supply and diversity. Because the state of technology readiness of biomass-sourced blendstocks is much less developed than conventional fossil-based blendstocks, we have analyzed 24 biomass-derived boosted SI blendstocks against 17 metrics assessing economic benefits, technology readiness, and environmental viability.[8] The findings of these analyses indicate that all of the top-performing blendstocks have the potential to reduce life-cycle greenhouse gas emissions by at least 60% compared to petroleum-based fuels. At a 30% blend level, this equates to an 18% reduction in emissions for the finished fuel. This information provides the biofuel community a comprehensive and consistent comparison of the feasibility and technical research and development barriers to commercializing promising boosted SI blendstocks.

Our research concludes that Co-Optima blendstocks have the potential to boost refinery profitability, even when considering a range of refinery sizes, locations, and complexities. When compared to traditional fossil streams, Co-Optima blendstocks would be valued by refiners at between \$2.40 to \$3.00 per gasoline gallon equivalent (GGE). This estimated value aligns closely with current DOE cost targets.

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[8] Dunn, J.B., M. Biddy, S. Jones, H. Cai, P.T. Benavides, J. Markham, L. Tao, et al. "Environmental, Economic, and Scalability Considerations and Trends of Selected Fuel Economy Enhancing Biomass-derived Blendstocks." *ACS Sustainable Chemical Engineering* 6(1):561–569. October 30, 2017. doi:10.1021/acssuschemeng.7b02871.

Bringing it all Together: Impacts on Engine Efficiency and Fuel Economy

The first three years of Co-Optima research have provided the technical foundation for industry to develop improved fuel/engine solutions by identifying fuel property impacts on engine efficiency, fuel blendstocks that are capable of providing those properties, and solutions that are scalable, sustainable, affordable, and compatible. Estimations indicate that fuel economy improvements are possible with improvements to RON, S, and HOV (see Figure 4).

Recent studies[9] suggest that high-RON, high-S fuels able to achieve these types of efficiency levels may be difficult to deploy at scale. To better understand options for improved fuel economy with more modest RON and S increases, current Co-Optima multimode efforts for passenger vehicles are exploring opportunities to significantly increasing part-load efficiencies via advanced compression ignition (ACI) approaches, with the goal of providing additional fuel economy benefits utilizing fuels that are deployable at scale.

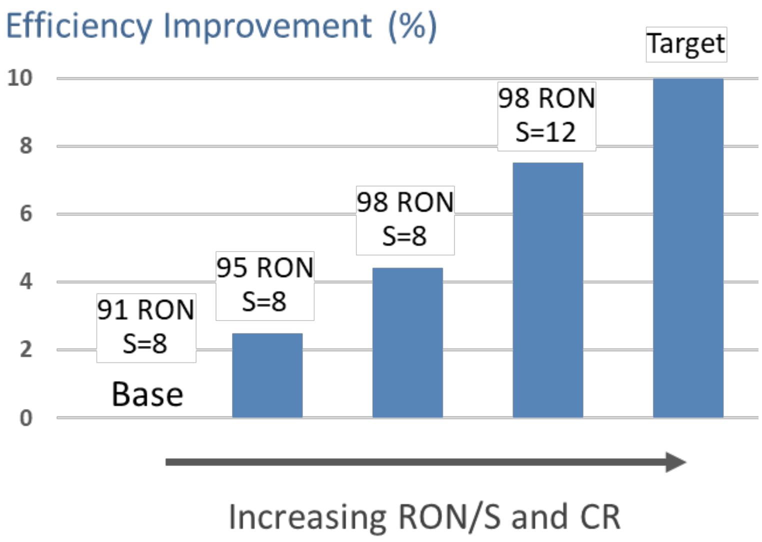

Figure 4. Estimations indicate that significant fuel economy improvements are possible with improvements to RON, S, and HOV.

Impacts across the fuel production, distribution, and retail sectors need to be balanced with those of the ultimate arbiter of the successful introduction of new fuels and engines—the consumer. The numerous sometimes competing priorities of these diverse stakeholders is a major reason why discussions related to advanced fuels and engines needs to be rooted in objective and rigorous science, engineering, analysis, and economics.

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[9] See for example "Analysis of the Potential for Increasing Octane in the U.S. Fuel Supply," Fuels Institute Report, 2018.

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