FY18

YEAR IN REVIEW

CO-OPTIMIZATION OF **FUELS & ENGINES**

U.S. DEPARTMENT OF ENERGY

Office of **ENERGY EFFICIENCY & RENEWABLE ENERGY**

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About The Co-Optimization of Fuels & Engines (Co-Optima) Initiative

The U.S. Department of Energy (DOE) Co-Optima initiative is accelerating the introduction of efficient, clean, affordable, and scalable high-performance fuels and engines. This first-of-its-kind effort is simultaneously tackling fuel and engine research and development (R&D) to maximize light-, medium-, and heavy-duty vehicle fuel economy and performance, while mapping lower-cost pathways to reduce emissions, leveraging diverse domestic fuel resources, boosting U.S. economic productivity, and enhancing national energy security.

Co-Optima brings together DOE's Office of Energy Efficiency & Renewable Energy (EERE), nine national laboratories, 13 universities, and numerous industry and government stakeholders in a collaboration exploring solutions with potential for near-term improvements to the types of fuels and engines found in most vehicles currently on the road, as well as potential for the development of revolutionary new engine technologies.

LETTER FROM THE LAB LEADERSHIP TEAM/EXECUTIVE SUMMARY

Innovation that will lead to better fuels and better vehicles while giving U.S. consumers new efficient, clean, and affordable transportation options has been the goal of our Co-Optima team from the initiative's launch. After three years of intensive collaborative research, spanning national laboratories and universities across the country, our scientists, engineers, and analysts are providing stakeholders with technical data, insights, and knowledge that could help catalyze dramatic change in the transportation landscape in the very near future and as time continues to unfold.

As researchers, we are taking an objective look at how integrated fuel, engine, and powertrain combinations can deliver co-optimized solutions that are more effective than the sum of their individual parts. Ultimately, industry leaders and policymakers will have access to the knowledge generated by Co-Optima to inform decisions regarding which changes could prove most viable and beneficial for drivers, businesses, and the environment. The resulting vehicle efficiency gains have the potential to save Americans tens of billions of dollars in annual fuel costs, and producing blendstocks from domestic biomass could boost the U.S. economy by creating jobs and keeping energy dollars in the United States.

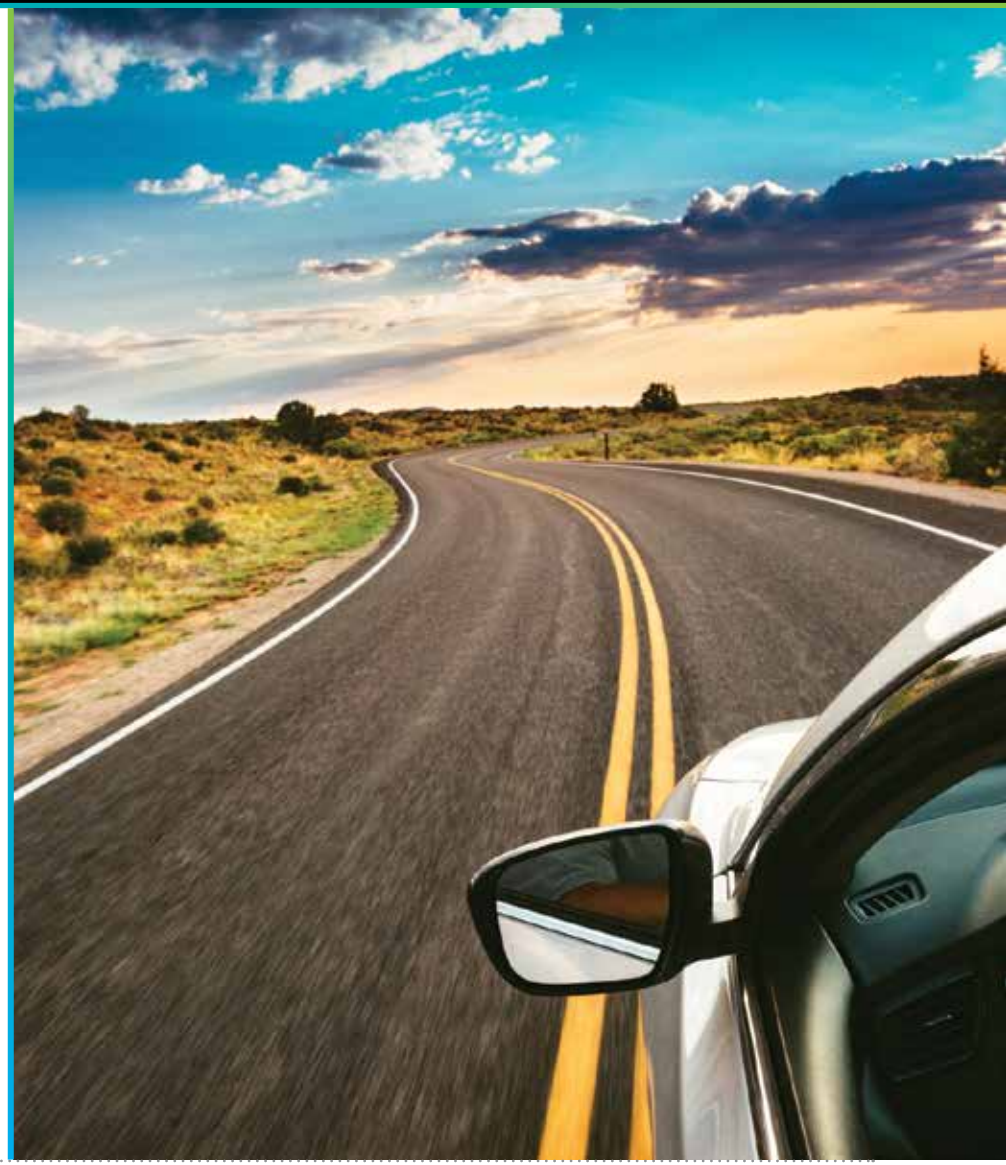
Fiscal Year 2018 (FY18) Co-Optima research culminated in the completion of research focused on full-time operation of downsized turbocharged (or "boosted") spark-ignition (SI) engines and fuels for light-duty (LD) vehicles. Discoveries addressing how fuel properties impact engine performance, which blendstocks offer desired fuel properties, and possible barriers to commercial introduction blaze a trail for new solutions, with the potential to dramatically increase passenger vehicle performance and efficiency.

As the boosted SI LD research neared completion, we ramped up research on multi-mode approaches that make use of a combination of SI and advanced compression ignition (ACI) methods to deliver even greater efficiencies for LD vehicles. Our team also continued to advance its understanding of mixing-controlled compression ignition and ACI regimes for medium-duty and heavy-duty vehicles.

This report spotlights these and other significant FY18 Co-Optima accomplishments including:

- Characterization of fuel properties and engine parameters capable of delivering a 10% increase in fuel economy for LD vehicles with boosted SI engines
- Identification of 10 blendstocks from four chemical families with the greatest potential to increase boosted SI efficiency and break down technical, economic, and environmental barriers to their near-term commercialization, including the six blendstocks with the fewest barriers
- Correlation of molecular structure with key fuel properties and metrics
- Creation of new computational tools to more rapidly identify new blendstocks and interpret data
- Establishment of modeling and analysis methods to characterize economic value and environmental performance across the supply chain
- Demonstration that autoignition performance of a broad range of fuels under ACI conditions correlates poorly with octane index, highlighting the need for new metrics.

The joint efforts of more than 100 researchers at partner labs and universities have been vital to these breakthrough achievements. We will welcome experts from new university and industry partners to the team in the coming year, and we will continue to rely heavily on guidance and input from stakeholders. Thanks to the vision and collaborative support of EERE's Vehicle Technologies Office and Bioenergy Technologies Office, we are propelling this vital research into the next stage.



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Oak Ridge National Laboratory

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Pacific Northwest National Laboratory

Chris Moen
Sandia National Laboratories

TECHNICAL RESEARCH ACCOMPLISHMENTS & IMPACT

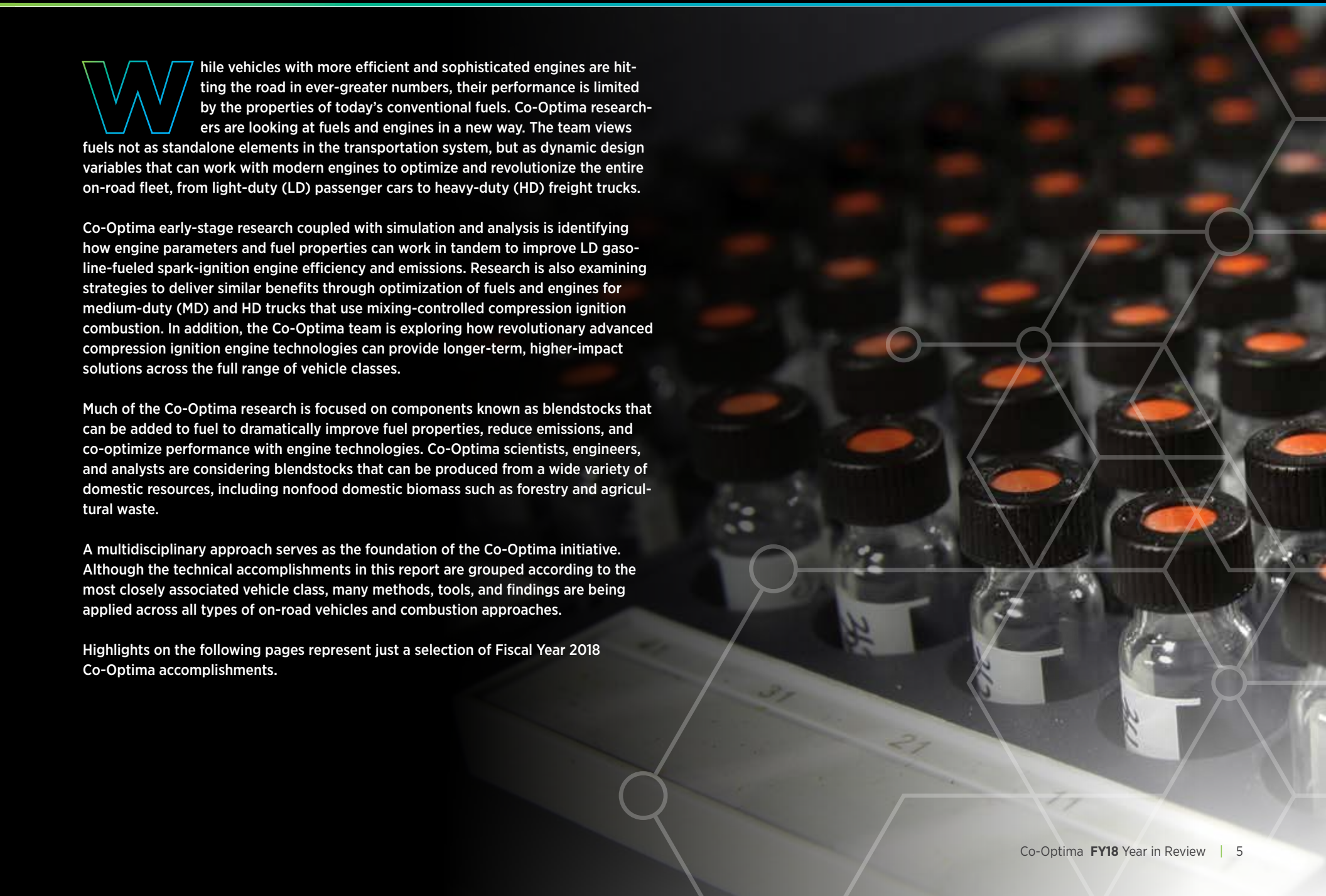
While vehicles with more efficient and sophisticated engines are hitting the road in ever-greater numbers, their performance is limited by the properties of today's conventional fuels. Co-Optima researchers are looking at fuels and engines in a new way. The team views fuels not as standalone elements in the transportation system, but as dynamic design variables that can work with modern engines to optimize and revolutionize the entire on-road fleet, from light-duty (LD) passenger cars to heavy-duty (HD) freight trucks.

Co-Optima early-stage research coupled with simulation and analysis is identifying how engine parameters and fuel properties can work in tandem to improve LD gasoline-fueled spark-ignition engine efficiency and emissions. Research is also examining strategies to deliver similar benefits through optimization of fuels and engines for medium-duty (MD) and HD trucks that use mixing-controlled compression ignition combustion. In addition, the Co-Optima team is exploring how revolutionary advanced compression ignition engine technologies can provide longer-term, higher-impact solutions across the full range of vehicle classes.

Much of the Co-Optima research is focused on components known as blendstocks that can be added to fuel to dramatically improve fuel properties, reduce emissions, and co-optimize performance with engine technologies. Co-Optima scientists, engineers, and analysts are considering blendstocks that can be produced from a wide variety of domestic resources, including nonfood domestic biomass such as forestry and agricultural waste.

A multidisciplinary approach serves as the foundation of the Co-Optima initiative. Although the technical accomplishments in this report are grouped according to the most closely associated vehicle class, many methods, tools, and findings are being applied across all types of on-road vehicles and combustion approaches.

Highlights on the following pages represent just a selection of Fiscal Year 2018 Co-Optima accomplishments.



> Clarifying Key Concepts

Co-Optima research relies upon, and is expressed in terms of, a number of key concepts related to efficiency, engine operation, and fuel properties. Many of these central theories, metrics, and processes are described in detail in subsequent sections focusing on specific vehicle classes and combustion regimes. The information in this section clarifies how overarching concepts of fuel economy, engine efficiency, and linear/nonlinear blending have been applied and interpreted in the course of Co-Optima research.

FUEL ECONOMY VS. ENGINE EFFICIENCY

Fuel economy reflects how far a vehicle can travel on a set amount of fuel, and is usually expressed in miles per gallon or miles per gasoline gallon equivalent (GGE). Miles per GGE is often used to provide a standard for comparing vehicle fuel economy for liquid fuels with different volumetric energy density (e.g., 85% ethanol blends) and with other fuels such as natural gas and electricity. While fuel economy depends on engine displacement, with high-efficiency engines typically providing greater vehicle fuel economy, it also relies on many other factors such as vehicle size, weight, powertrain (type of transmission, extent of hybridization), and drive cycles (city vs. highway driving).

In contrast, engine efficiency focuses specifically on the engine and is a measure of how efficiently the engine converts fuel energy into mechanical work (e.g., to move the vehicle). Measured as a percentage, it depends on engine parameters (such as compression ratio), as well as operating conditions (speed and load). Engine efficiency is typically the metric of interest in fundamental fuel/engine studies due to its reliance on measurements related directly to engine operation, rather than other vehicle characteristics (transmission, vehicle size, etc.). By concentrating on this metric, researchers are able to more accurately evaluate the potential for fuel-engine co-optimization.

LINEAR VS. NONLINEAR BLENDING

The behavior of a blendstock when combined with a petroleum base fuel can strongly impact performance of the finished fuel. Fuel properties can behave in a linear, synergistic nonlinear, or antagonistic nonlinear fashion following blending. Understanding these behaviors is vital to successful formulation of new high-performance fuels.

When properties blend in an approximately linear fashion, the properties of the resulting fuel can be readily calculated based on a simple linear combination of the properties of its components. For example, the heat of vaporization (HOV) of a fuel is roughly equal to the sum of the HOV of each component, weighted by its concentration in the final blend. In the case of a 50:50 blend of two blendstocks, the HOV of the finished fuel would be approximated by the following equation:

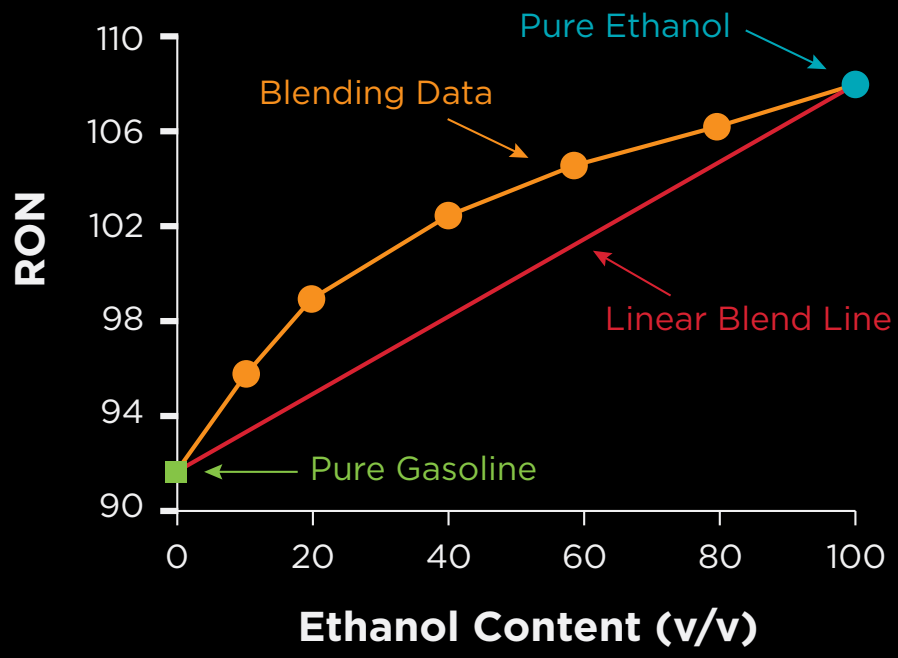
HOV (fuel blend) = 0.5 x HOV (blendstock 1) + 0.5 x HOV (blendstock 2)

Some important fuel properties—in particular research octane number (RON), motor octane number (MON), and the difference between the two (S)—blend nonlinearly. Nonlinear behavior results in fuel properties that are either higher (synergistic in the case of RON, MON, and S) or lower (antagonistic) than a linear calculation would predict.

For example, the RON of an ethanol and gasoline mixture is greater than would be predicted based on linear blending assumptions, as shown in the figure.

Ethanol exhibits synergistic nonlinear blending for RON—the RON of the blend is greater than predicted based on linear blending assumptions, and this enhanced RON is advantageous from a performance perspective. Alcohols in general exhibit synergistic nonlinear blending for RON, as do other blendstock families such as furans, olefins, and cyclic ketones.

Esters, conversely, exhibit antagonistic nonlinear blending—the RON of the blend is lower than the RON predicted based on linear blending assumptions. This means that blending an ester into a base fuel to achieve a target RON increase requires larger concentrations than use of an alcohol with the same RON value would require.



RON data for pure gasoline, pure ethanol, and gasoline/ethanol blends. The red line shows the RON expected if ethanol blended linearly with gasoline.

RUNNING THE NUMBERS: NEW METHODS, GREATER ACCURACY

Highlights throughout this section describe improved methods of measurement and assessment that capture the interplay of new fuels and combustion approaches better than established techniques. Co-Optima research shows that RON, MON, octane index, particulate matter index, and many other standard diagnostic benchmarks by themselves fall short of the mark in accurately predicting performance of new fuels and engines when advanced compression ignition combustion approaches are used. As a result, the Co-Optima team is developing alternative protocols and metrics that are capable of more reliably and precisely characterizing impacts of fuel properties on engine operation.

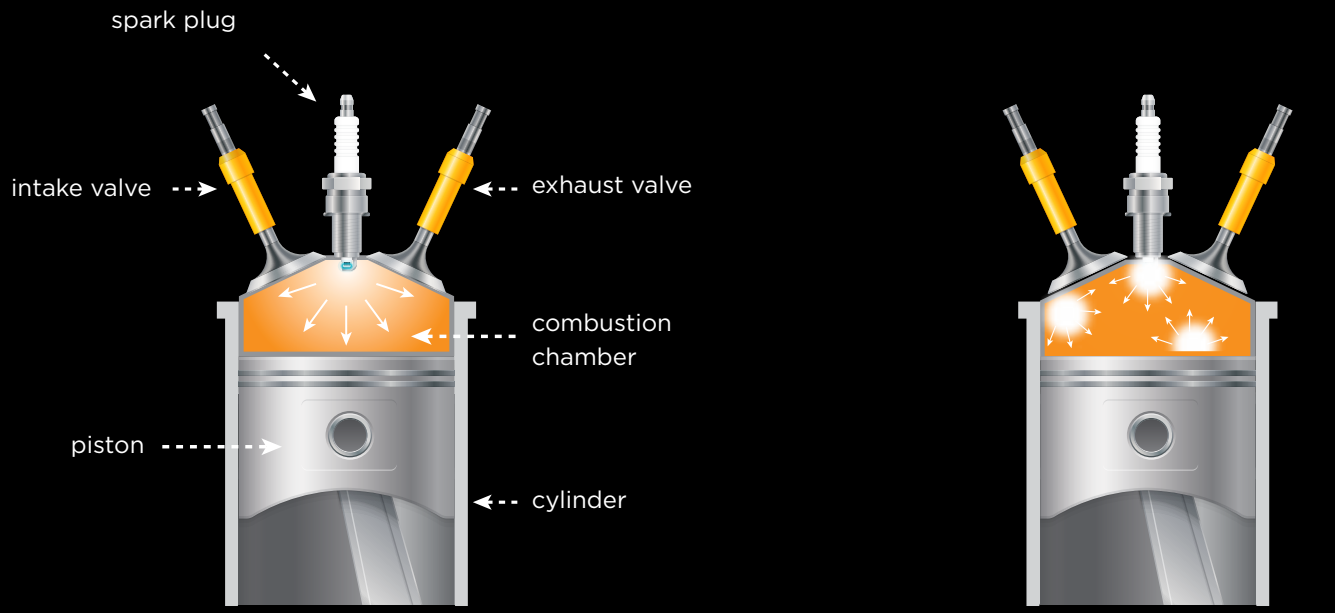
> Light-Duty Vehicle Landmark: Completion of Boosted SI Research

MAXIMIZING EFFICIENCY, MITIGATING KNOCK

Manufacturers are increasingly introducing vehicles with downsized turbocharged (or "boosted") spark-ignition (SI) engines that deliver higher power density and improved fuel economy. However, the very characteristics that maximize efficiency in these boosted SI engines also exacerbate damaging autoignition or "knock"—the spontaneous ignition of fuel triggered by high temperatures and pressures inside engine cylinders.

In Fiscal Year 2018 (FY18), the Co-Optima initiative completed its research focused on full-time boosted SI operation, much of which concentrated on identifying the fuel properties and engine parameters needed to maximize boosted SI efficiency and performance in light-duty (LD) vehicles.

Normal Combustion vs. Knock



Normal flame propogation
Unburned fuel/air mixture combusts once flame front reaches it

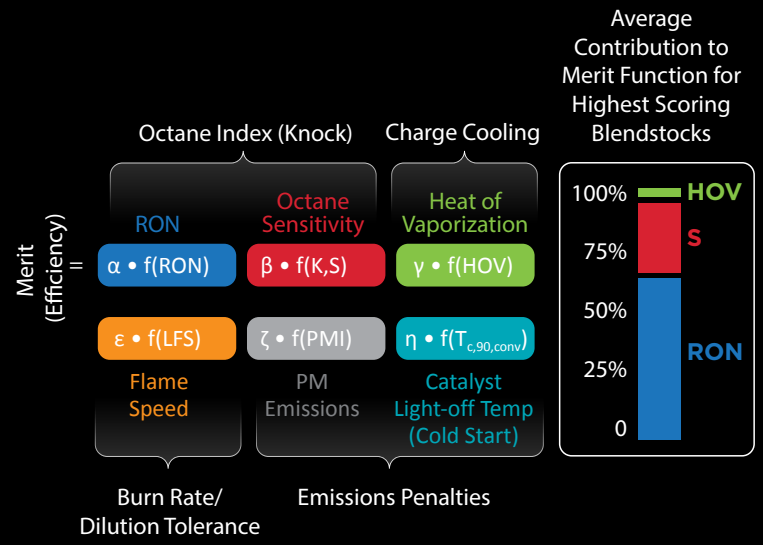
Knock
Unburned fuel/air autoignites before flame reaches it

Engine knock caused by spontaneous ignition of the unburned fuel/air mixture is promoted by increased temperature, pressure, and time.

PINPOINTING FUEL PROPERTIES FOR OPTIMAL PERFORMANCE

Co-Optima research and analysis identified the fuel properties needed for optimal operation of boosted SI LD engines through development of a merit function. Because the merit function predicts 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 common metrics such as anti-knock index which do not relate directly to engine efficiency. The merit function quantifies the impact of six fuel properties—research octane number (RON), octane sensitivity (S), heat of vaporization (HOV), flame speed, particulate matter index (PMI), and catalyst light-off-temperature—on boosted SI efficiency. It represents the most detailed correlation to date of fuel properties and engine efficiency. The distinct algebraic form of the merit function has the unique attribute of being able to assess the tradeoffs between the impact of different fuel properties, revealing how to meet the same efficiency target through different combinations of fuel properties. For example, a decrease in RON can be offset by increasing S.

Boosted SI Merit Function Showing Individual Terms That Contribute to Engine Efficiency



The righthand bar shows the average contribution of RON, S, and HOV to the overall merit function score for eight of the highest scoring boosted SI blendstocks. Contributions from the other three terms—flame speed, particulate matter (PM) emissions, and catalyst light off temperature—are small under boosted SI operating conditions for most blendstocks.

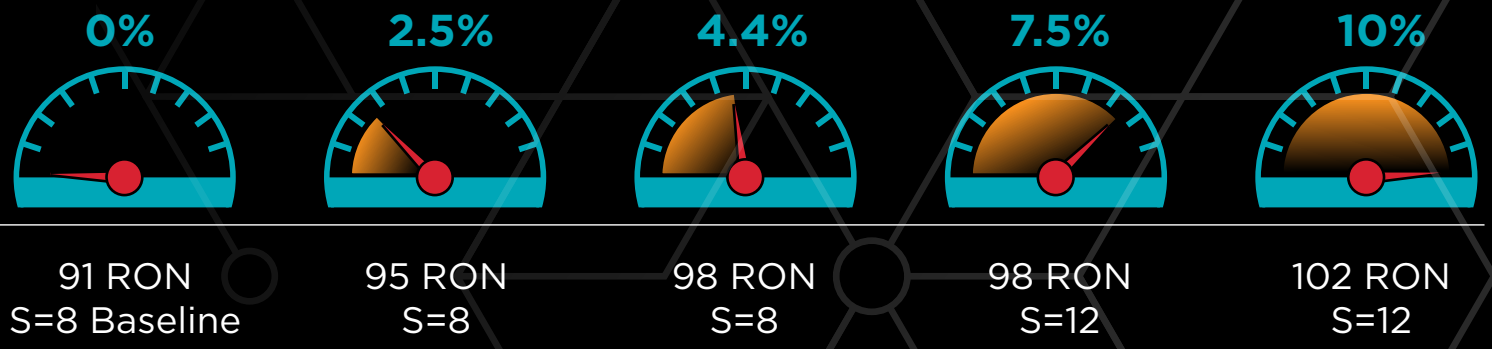
Efforts during FY18 focused on refining Co-Optima fuel property data and blending models, conducting experiments to improve the team's understanding of fuel property impacts on engine performance, and addressing key scientific lines of inquiry, such as the nature of nonlinear octane blending. Key findings indicate that:

- RON, S, and HOV are the fuel properties with the most consistently significant impact on boosted SI engine efficiency.
- RON and S can provide benefits well beyond those of HOV.
- The contribution to the merit function score (debit) from the PMI term is small for most blendstocks, except for highly aromatic candidates such as biorefor-mate.

The research team demonstrated that fuels with higher RON, S, and HOV not only contribute to engine efficiency improvements, but can improve boosted SI engine fuel economy by up to 10%.

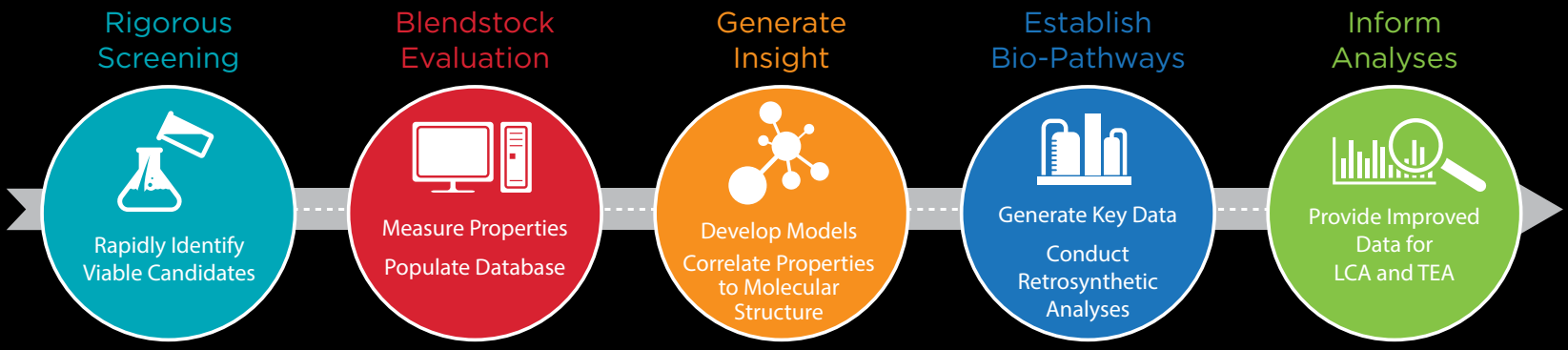
This work has supplied a new fundamental understanding of how in-cylinder temperature, pressure, mixture composition, and fuel kinetics impact knock and engine efficiency. In addition, it has provided a fresh look at how fuel properties, engine parameters, and fuel composition interact to produce PM.

Merit Function Estimates of Boosted SI Engine Efficiency Increase



Merit function estimates of boosted SI engine efficiency increase associated with changes in fuel RON and S. Efficiency benefits of 10% are predicted to be feasible, though the high RON/S fuels required would be expensive and difficult to deploy at scale.

Blendstock Screening Process



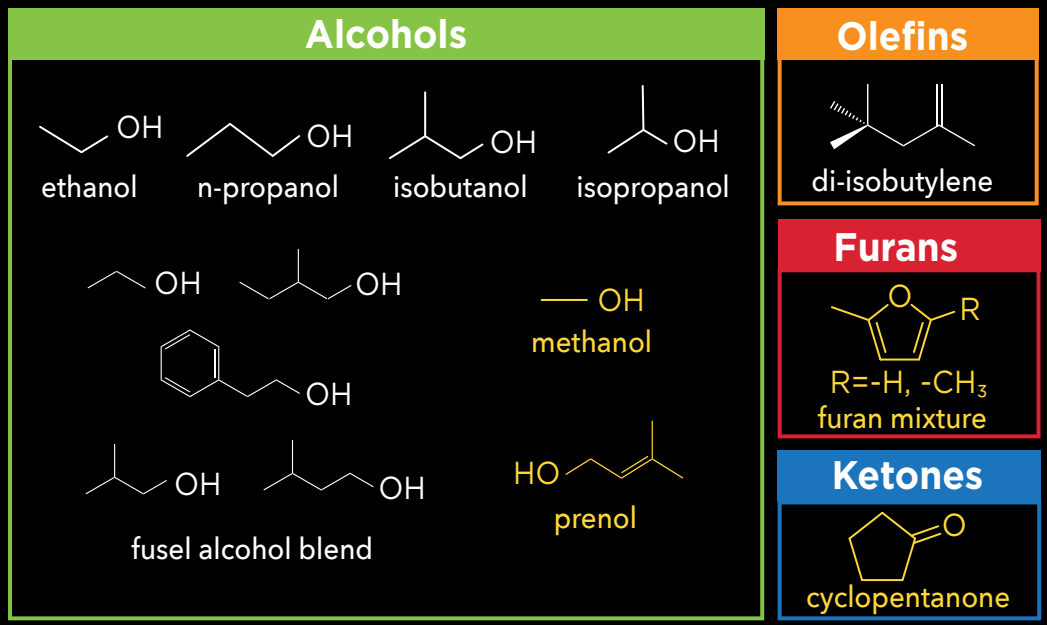
Overview of process used to screen, identify, and analyze high-potential Co-Optima blendstocks. LCA = Life cycle analysis. TEA = techno-economic analysis.

IDENTIFYING BLENDSTOCKS WITH THE GREATEST POTENTIAL FOR IMPROVING BOOSTED SI PERFORMANCE

Building on Co-Optima's systematic FY17 study of more than 400 potential blendstocks, researchers provided additional insights into the fuel properties imparted by 14 chemical families to help identify new fuels for boosted SI engines. Rigorous screening and evaluation have identified 10 blendstocks from four chemical families that have been determined to have the greatest potential to increase boosted SI engine efficiency.

Small alcohols are the only chemical family that can impart significant improvements to all three key boosted SI fuel properties (RON, S, and HOV). These blendstocks can be produced from resources including renewable domestic biomass, resulting in significant reductions in greenhouse gas (GHG) emissions. Co-Optima researchers have assessed optimal production pathways for bio-derived fuels, potential emissions-control systems impacts, materials compatibility issues, and a wide range of technological, economic, and environmental factors related to these blendstocks.

Blendstocks with Highest Merit Function Scores:

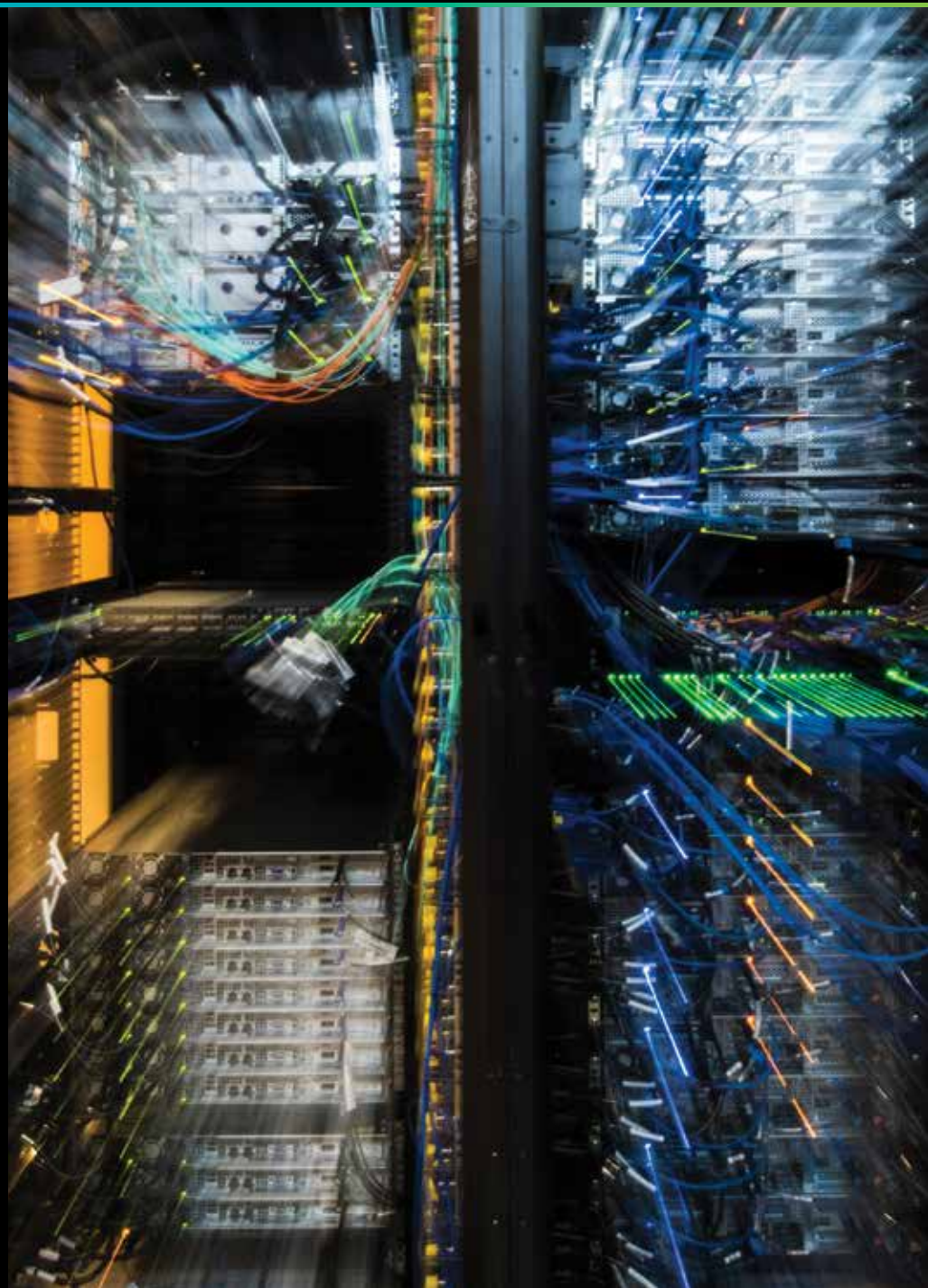


Ten blendstocks from four chemical familes with the greatest potential to increase boosted SI engine efficiency (as determined by merit function scores). The assessment found the six blendstocks in white had the fewest significant barriers to adoption.

ACCELERATING R&D WITH NEW STATE-OF-THE-ART TOOLS

Many FY18 accomplishments and the accelerated pace of Co-Optima research and development (R&D) were made possible by the team's development of new capabilities, numerical algorithms, and computational tools. For example, a high-throughput, constant-pressure spray chamber was designed and constructed to measure spray dynamics under conditions that simulate engine thermodynamic conditions at the time of fuel injection.

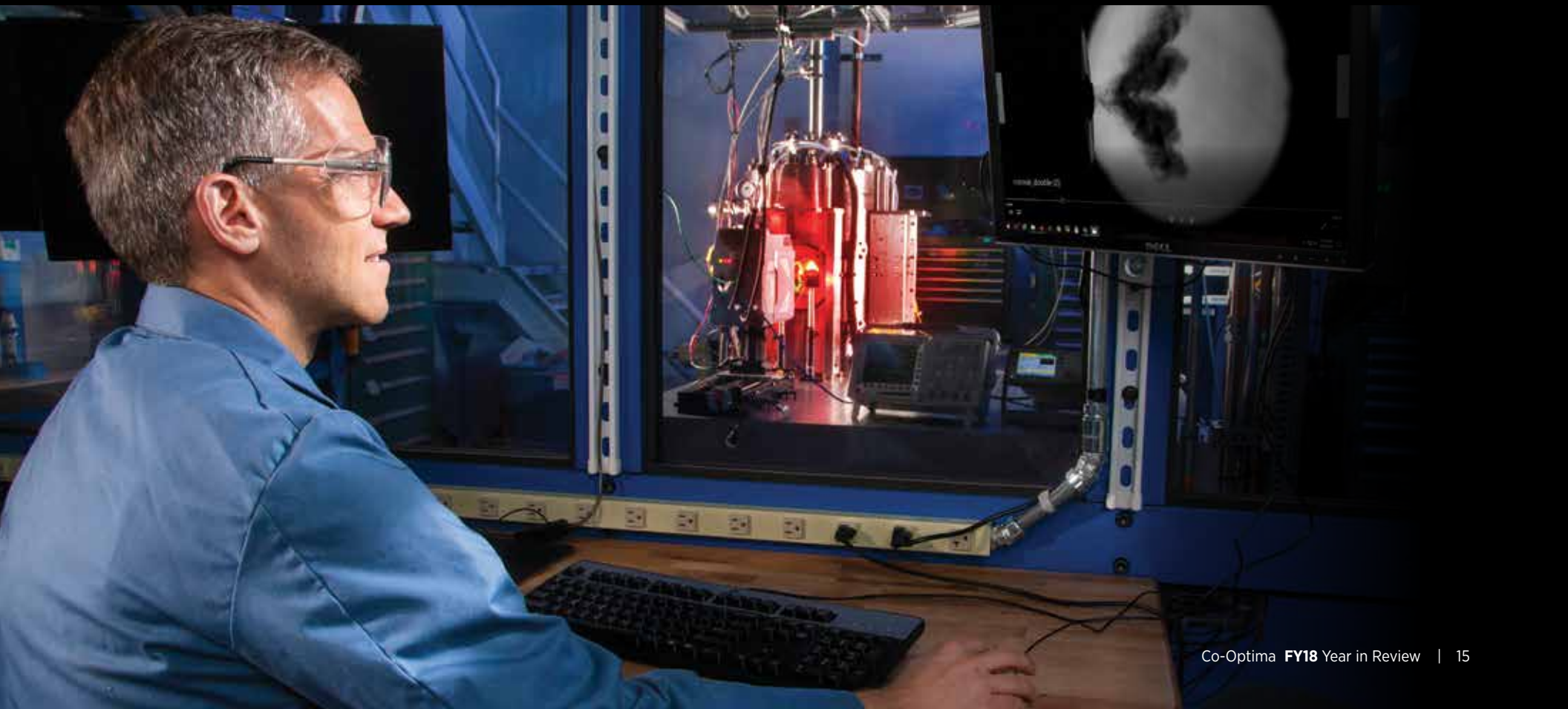
The Co-Optimizer software tool has been refined, giving researchers and stakeholders the ability to assess candidate blendstocks in relation to tradeoffs involving a number of complex variables, including production scale and economics, life-cycle emissions, and infrastructure compatibility. Another tool allows researchers to quickly generate surrogate fuel mixtures to match key physical and kinetic properties for use in fuel and engine simulations. A number of additional tools have been developed to estimate a wide range of fuel properties based on chemical structures, enhancing researchers' ability to rapidly screen for the most promising candidates. Also, a continuously updated fuel property database makes Co-Optima data readily accessible to researchers nationwide (https://fuelsdb.nrel.gov/fmi/webd/FuelEngine-CoOptimization). Once development is complete, all Co-Optima tools will be made available online to stakeholders.



TRANSITIONING TO MULTIMODE RESEARCH

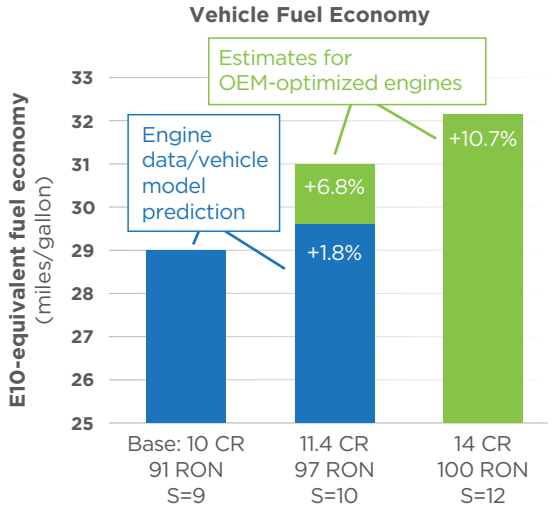
As the team pushes into FY19, Co-Optima LD R&D is transitioning to focus more intently on multimode combustion approaches, which have the potential to deliver even greater efficiency and cost savings by using different methods of ignition, combustion, and/or fuel-preparation depending on driving demands. While Co-Optima has identified how to achieve efficiency targets using a boosted SI approach, analyses by external organizations indicate that the required properties may result in fuels that are expensive and difficult to deliver at a large scale. This has led Co-Optima researchers to build on their boosted SI understanding and concentrate on multimode fuel-engine approaches with the potential to cost-effectively achieve the 10% Co-Optima fuel efficiency goal. Researchers are exploring multimode lean SI, lean advanced compression ignition (ACI), and dilute stoichiometric ACI approaches, along with the related fuel properties needed to maximize efficiency and emissions.

More details on select Co-Optima FY18 accomplishments related to LD vehicles can be found in the following section.



Vehicle Simulations Show Pathway for Blendstocks & Optimized Engines to Increase Fuel Economy

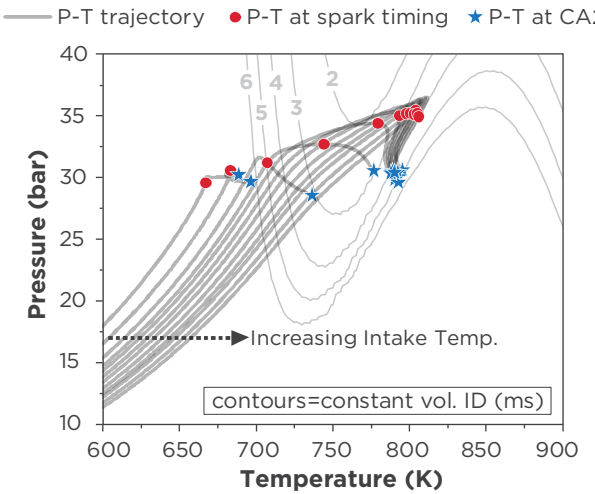
Optimizing engine operation to exploit improved fuel properties is a central Co-Optima goal. Researchers studied the ability of high-performance blendstocks to improve turbocharged, direct-injection SI engine efficiency and fuel economy. The study used results of multicylinder engine experiments, Co-Optima merit function predictions, fuel blend analyses, and vehicle simulations. It projected that six candidate blendstocks—ethanol, n-propanol, isopropanol, isobutanol, diisobutylene (DIB), and a bioreformate surrogate—could improve engine efficiency and increase E10-equivalent fuel economy by as much as 12% at blend levels up to 35%. Of these, the blendstock that provided the highest efficiency benefit at a given blend level (neglecting real-world considerations such as infrastructure impacts, blend challenges, and market factors) was ethanol, due to its ability to provide large improvements in RON, HOV, and S. Vehicle simulations using experimental data from a boosted SI engine optimized for RON 97 and S 10 indicated that E10-equivalent fuel economy could be improved by 1.8% compared with the same vehicle using today's E10 gasoline with RON 91 and S 9. (E10 is gasoline containing 10% ethanol.) Estimates indicated that the fuel economy could be increased by up to 6.8% on an E10-equivalent basis with additional engine optimization and up to 10.7% in a fully optimized engine with a compression ratio (CR) of 14 operating with RON 100/S 12.



E10-equivalent fuel economy for base engine/conventional E10 fuel (RON 91, S 9, HOV 415 kJ/kg), 11.4 CR engine/RON 97 fuel (S 10, HOV 479 kJ/kg), and 14 CR/RON 100 (S 12, HOV 517 kJ/kg). Blue bars represent fuel economy based on engine data and vehicle simulations. Green bars represent further improvements possible through original equipment manufacturer (OEM) optimization (e.g., piston geometry, fuel injector design). Fuel economy improvements greater than 10% are possible with high engine CR and very high RON/S/HOV fuels. Figure by Scott Sluder, ORNL

Pre-Spark Heat Release May Provide a Means to Mitigate Engine Knock

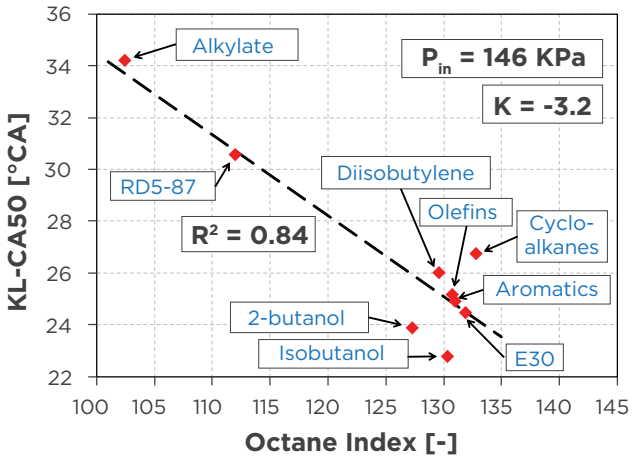
Mitigating engine knock through fuel and engine approaches is critical for improving engine efficiency and fuel economy in boosted SI engines. Analysis of cylinder pressure traces demonstrated that engine operating conditions that promote pre-spark heat release (PSHR) alter the traditional intake temperature-knock relationship—allowing more advanced knock-limited combustion phasing, provided that the fuel has significant negative temperature coefficient (NTC) behavior. The cause for this behavior is believed to be that, with sufficient PSHR, the increased unburned gas temperature moves the thermodynamic state through the NTC region and into a long-ignition-delay region, as shown in the figure. This process results in near-isobaric heat addition, where significant changes in ignition delay and fuel composition occur. The findings suggest that low-temperature heat release processes are likely present in the end gas of SI engines, but that they are not readily observable with conventional pressure-based combustion diagnostics. Fuel properties such as S and kinetics were observed to reduce the sensitivity of PSHR and knock to intake temperature and therefore expand the operational window of PSHR-prone fuels, leading to an increase in engine efficiency. This also indicates that, for some fuels, PSHR could offer benefits for knock-limited engine operation and associated effects on abnormal combustion under conditions relevant to downsized, boosted SI engines.



Pressure-temperature trajectory up to 2% of heat release (CA2) of the deflagration (blue stars), with spark-discharge timing denoted (red circles) for an intake temperature sweep with boosted operation at 2,000 revolutions per minute (rpm). The engine data are plotted on constant-volume ignition-delay simulation results in milliseconds (gray numbers), with ignition delay defined as a 50 K temperature rise. Figure by Derek Splitter, ORNL

Iso- & 2-Butanol Fuel Blends Produce Less Knock Than Expected Under Load-Transient Boosted Conditions

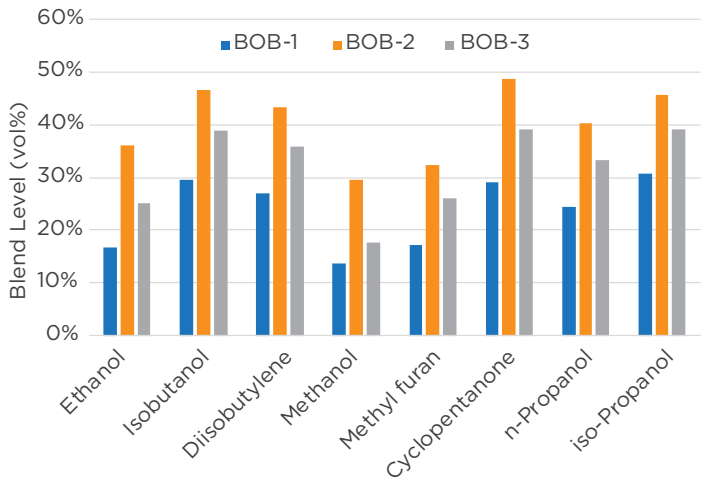
Results of direct-injection SI engine experiments conducted to map knock limits highlighted inconsistencies in reliance on RON and motor octane number (MON) metrics. These findings imply that the true knock performance of new fuels must be carefully assessed prior to market introduction. Researchers examined eight RON 98 fuels of varying composition and S, as well as one representative regular E10 gasoline (RD5-87). These fuels were evaluated over a wide range of engine intake pressures and thermal states for various well-mixed stoichiometric engine-operating strategies, including steady and load-transient operation. For cooler, boosted, load-transient operation—resulting in K values much more negative than typical of representative boosted SI operation (K = -3.2 vs. -1.25)—significant deviations from the octane index (OI) correlation were observed. The K-factor is specific to each operating condition and notionally relates the operating conditions to those of the RON and MON tests. Monte Carlo uncertainty modeling indicated a high likelihood of real chemical fuel effects causing isobutanol and 2-butanol fuel blends to be less knock-limited and cycloalkanes to be more knock-limited, compared with expectations based on their OIs.



Correlation between knock-limited combustion phasing and OI, revealing deviations for some fuels under load-transient boosted SI engine operation. Knock limits were plotted against the OI computed from each fuel's RON and MON, with OI = RON-K (RON-MON). KL-CA50 indicates the combustion phasing that causes a predetermined knocking threshold to be met; lower KL-CA50 values indicate that a fuel is less knock-limited. Figure by Magnus Sjöberg and David Vuilleumier, SNL

Eight Bioblendstocks Demonstrate Strong Efficiency Improvements at Moderate Blend Levels

Previous Co-Optima analyses projected that substantial reductions in fossil energy consumption and GHG emissions from transportation would accrue slowly if biofuels were blended with gasoline at levels above 50% because ramping up biofuel production capacity to satisfy that level of blending would take decades. Consequently, Co-Optima researchers and analysts are focused on identifying blendstocks that can provide the greatest performance benefits at the lowest blending volumes. Using the Co-Optima merit function—a numerical relationship developed to quantify the association between fuel properties and boosted SI engine efficiency in co-optimized engines—researchers identified the blend levels required for 21 bioblendstocks to achieve an estimated 10% engine efficiency improvement when combined with current blendstocks for oxygenate blending (BOBs) used to blend commercial E10 regular (87 anti-knock index [AKI]) gasoline. Of these 21 bioblendstocks, eight met the efficiency target below 50% blending. Isopropanol and the furan mixture were subsequently selected for further analysis of transportation-sector-level benefits available from wide-scale deployment, due in part to their differing production routes and compatibility with gasoline storage and distribution infrastructure, two factors that influence cost and environmental impacts. Analysis results will be released in the next FY.



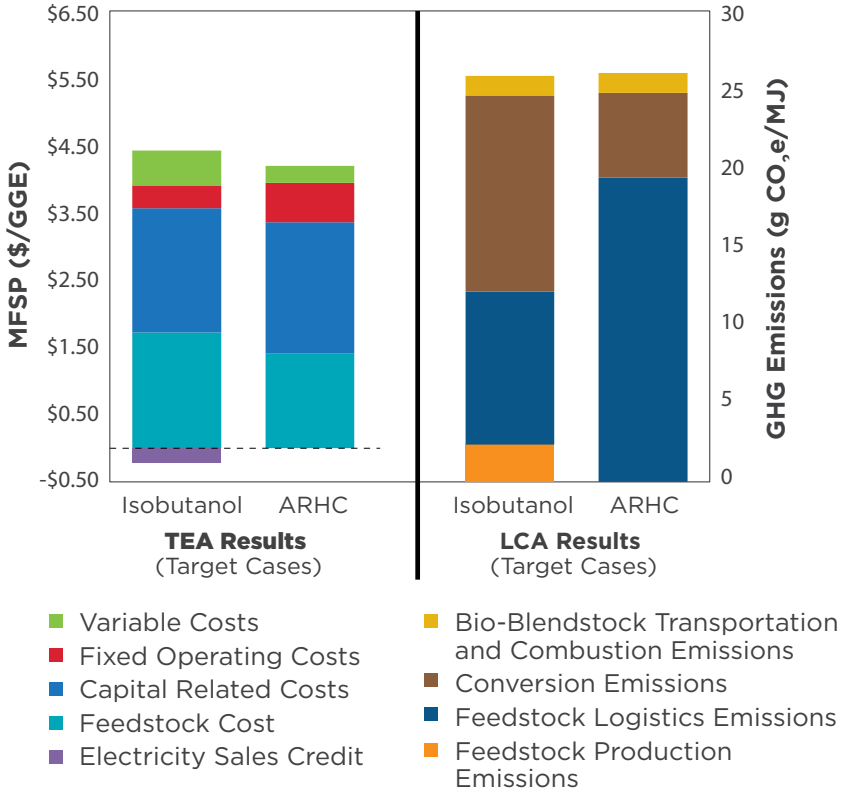
Blending levels (with different BOBs used to blend commercial E10 regular gasoline) for different bioblendstocks that achieve a 10% engine efficiency gain. Figure by Jennifer Dunn, ANL

Seven Bioblendstocks Show Potential to Meet Cost Targets

The cost-competitiveness of new bioblendstocks depends strongly on their ability to impart beneficial properties to fuels as well as flexibility and utility to fuel providers. Using tools and methods that align with petroleum refiners' economic evaluations, Co-Optima analysts assessed the economic value of seven bioblendstocks for boosted SI engines to petroleum refiners based on the most desirable blendstock properties. For the seven bioblendstocks considered, strongly nonlinear and synergistic octane blending translated into opportunities to improve petroleum refining economics. For a representative petroleum refinery configuration and performance, all seven blendstocks would be valued by refiners at prices that align closely with the current DOE Bioenergy Technologies Office long-term biofuel cost target of $2.50/gasoline gallon equivalent (GGE).

Analyses of Isobutanol & ARHC Reveal Potential for Economic Viability, Reduced Emissions

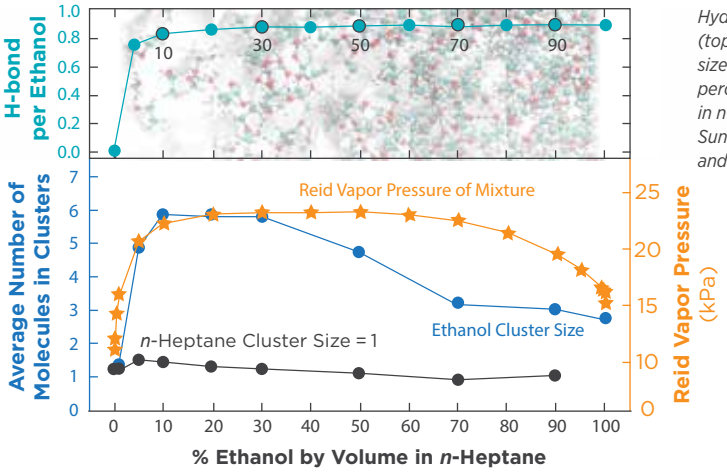
Isobutanol and aromatic-rich hydrocarbons (ARHC) are bioblendstocks with beneficial properties that could increase efficiency when blended into fuels used in optimized SI engines and, produced with biochemical and thermochemical conversion technologies, respectively, are reasonably mature in terms of commercial readiness. The Co-Optima team conducted detailed techno-economic analysis (TEA) and life-cycle analysis (LCA) to evaluate technology readiness, economic viability, and environmental impacts of these blendstocks. The minimum estimated fuel selling price (MFSP) of isobutanol ranged from $5.57/GGE based on today's technology to $4.22/GGE with technology advancements. The MFSP of ARHC could decline from $5.20/GGE based on today's technology to $4.20/GGE as technology improves. Both isobutanol and ARHC offer GHG emission reductions of about 73% relative to petroleum gasoline. On the other hand, production-related water consumption as well as life-cycle nitrogen oxide and fine PM ($PM_{2.5}$) emissions related to bioblendstock production logistics exceed the levels associated with petroleum gasoline. Improving the efficiency of and decreasing emissions from agricultural equipment used to cultivate feedstocks, along with process engineering to reduce water needed for production, could ameliorate negative impacts and reduce the life-cycle pollutant emissions of these bioblendstocks.



Detailed results of TEA and LCA for isobutanol and ARHC. CO_2e = carbon dioxide equivalent. Figure by Hao Cai, ANL

Study Illuminates Impact of Molecular-Level Aggregations on Fuel Properties

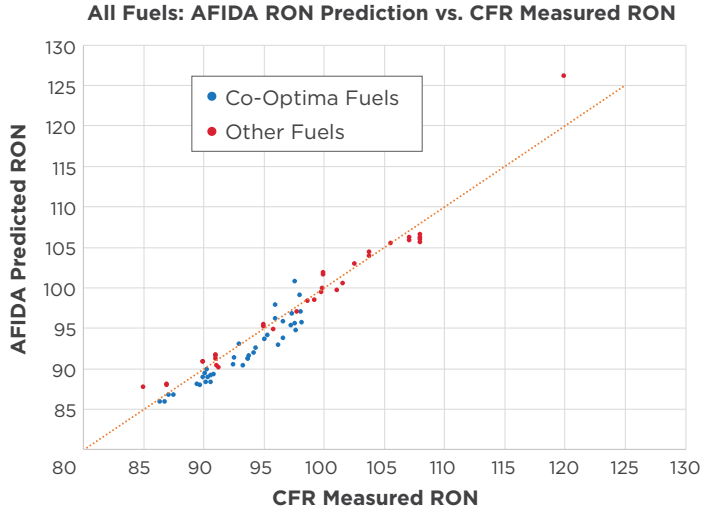
A key focus of Co-Optima fuels research has been improving fundamental understanding of blending relationships between key fuel chemical and physical properties, especially for oxygenated blendstocks, which have been studied much less than petroleum-derived hydrocarbons have been. Researchers showed that molecular-level aggregations within complex gasoline mixtures may influence critical properties for fuels containing polar blendstocks. Nuclear magnetic resonance (NMR) diffusion measurements and molecular dynamics simulations were used to understand competition between molecular cluster and hydrogen-bonding network formation in gasoline surrogates consisting of ethanol in n-heptane or iso-octane. The data indicate that, although discrete ethanol clusters are present at very low ethanol concentrations, fully developed hydrogen bonding networks dominate at concentrations of 10% ethanol (by volume) and higher. Increases in Reid vapor pressure (RVP)—a measure of gasoline volatility—corresponded to the size and number of ethanol clusters, while decreases in RVP paralleled the extent of the hydrogen-bonding networks. Additional work will examine the clustering of ethanol, isobutanol, and other oxygenates to clarify the fundamental processes governing RVP in multicomponent and complex fuels, which have significant cost implications for fuel producers.



Hydrogen-bonding networks (top) and ethanol cluster size and RVP (bottom) vs. percent ethanol by volume in n-heptane. Figure by Kee Sung Han, Amity Andersen, and Rose Perry, PNNL

Rapid, Low-Volume Octane Estimation Method Accelerates the Characterization of Boosted SI Fuels

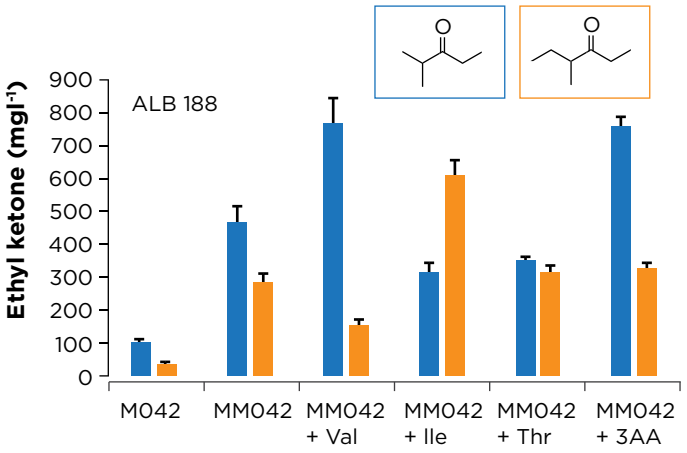
One of the major barriers facing fuels researchers is obtaining reliable estimates of fuel ignition properties for promising blendstock candidates when only low quantities are available. For example, traditional RON testing requires 500 ml of fuel and can take several hours to run. Co-Optima researchers demonstrated the ability of the Advanced Fuel Ignition Delay Analyzer (AFIDA)—a simplified bench-scale combustion device that correlates ignition delay with fuel metrics—to quickly generate accurate RON estimates in less than an hour and with a sample of less than 40 ml. When validated against results from a Cooperative Fuels Research (CFR) engine, the AFIDA estimated RON with less than 2% error (85–110 RON) for a broad range of fuels, spanning 65 oxygenated blendstocks in base fuels from simple surrogates to full-boiling-range gasolines. The researchers also demonstrated the AFIDA's ability to estimate S within brackets (low, medium, high). In addition, the AFIDA's flexible capabilities have proved useful for analysis of diesel- and gasoline-range blends, in particular estimates of indicated cetane number and parametric ignition delay mapping for validation of kinetic mechanisms.



AFIDA-predicted RON vs. RON measured on the CFR engine, showing excellent agreement. Red points are oxygenated blends in primary reference fuels, toluene standardization fuels, and complex gasoline surrogates. Blue points are oxygenated candidates blended into the core Co-Optima boosted SI fuels. Figure by Jon Luecke, NREL.

New Platform Based on PKS Enzymes Boosts Biochemical Production of Novel Bioblendstocks

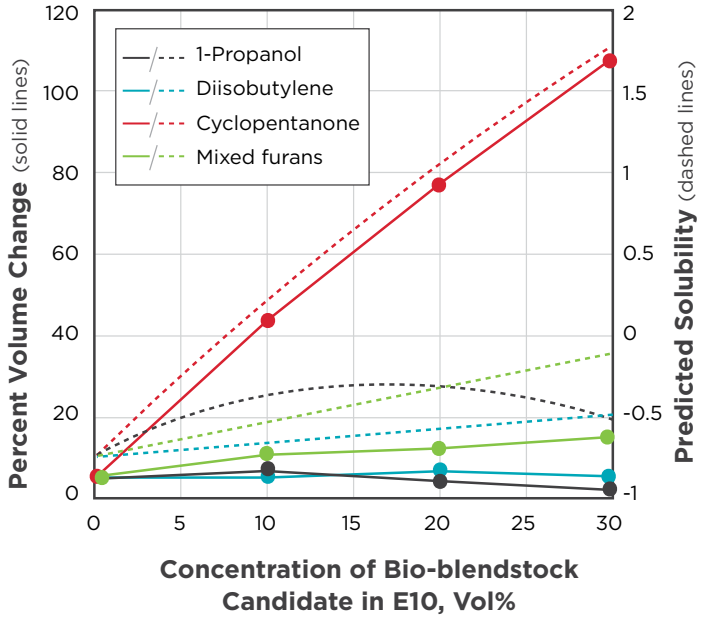
New diverse synthesis routes are required to improve the economics, environmental benefits, and scalability of novel bioblendstocks. Researchers developed a new platform for biochemical fuel production with tailored autoignition and thermophysical properties based on metabolic engineering of modular polyketide synthase (PKS) enzymes. Although modular PKS enzymes produce an enormously diverse group of molecules in nature, to date their complexity has stymied metabolic-engineering efforts. The researchers overcame this barrier by engineering a PKS system into the native host bacterium Streptomyces albus and optimizing cultivation conditions, including both carbon and nitrogen sources. Using this approach, they demonstrated production of over 1 g of six-carbon (C6) and seven-carbon (C7) ketones per liter of cellulosic hydrolysates—representing a 200-fold improvement over previous efforts. This flexible platform could enable biosynthesis of an array of previously inaccessible molecules, allowing fine-tuning of boosted SI fuel properties. This platform also holds the promise of producing diesel-range biofuels with superior ignition, emissions, and cold-weather performance.



Final titers of C6 and C7 ethyl ketones with Streptomyces albus strain ALB188, in standard growth medium M042 and in more concentrated growth medium MM042. Amino acids supplemented include valine (Val), isoleucine (Ile), threonine (Thr), and all three acids in combination (3AA). Varying amino acid supplements enables controlled production of shorter- or longer-chain ketones. Figure by Eric Sundstrom, LBNL

Exposure Studies Confirm Three Blendstocks' Compatibility with Vehicle & Fueling-Infrastructure Materials

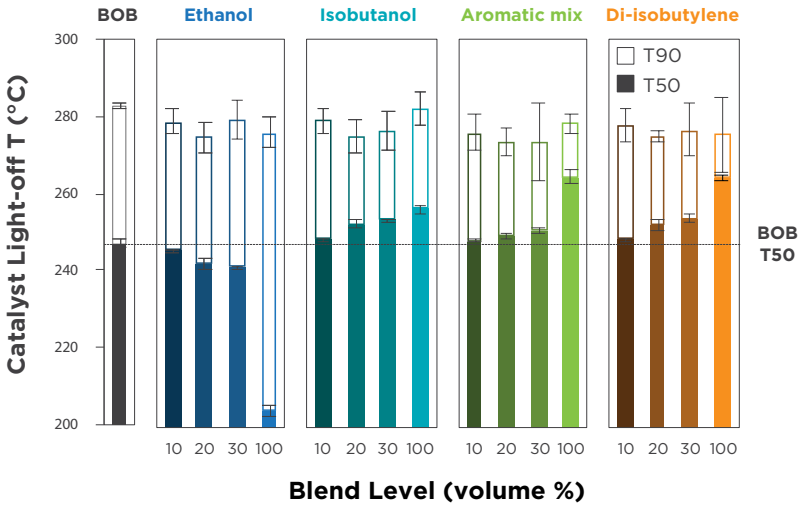
One of the largest barriers to introducing new blendstocks is potential incompatibility with materials found in legacy vehicles, fuel distribution equipment, and retail fueling hardware. Consequently, Co-Optima researchers have been evaluating the compatibility of promising blendstocks with materials commonly used in vehicles and fueling infrastructure. Researchers used exposure studies to confirm compatibility predictions for four boosted SI blendstock candidates—1-propanol, DIB, cyclopentanone, and mixed furans—mixed with E10 at levels of 10%, 20%, and 30% by volume. They applied these fuels to fluorocarbon elastomers that are used extensively in fuel storage and dispensing systems as well as in onboard vehicle fueling systems, and they measured the changes in the volume of the elastomers. The results showed that 1-propanol, DIB, and furans are compatible with the elastomers, while cyclopentanone causes excessive swelling. These results are consistent with predictions based on the solubility of the elastomers in these fuels. The results highlight the utility of solubility analysis for predicting fuel compatibility and the importance of experimentally confirming fuel candidates' compatibility with existing materials.



Percent volume change of fluorocarbon elastomer vs. concentration of blendstock candidates in E10 (solid lines, left axis), and Hansen solubility prediction (dashed lines, right axis). Figure by Mike Kass, ORNL

Boosted SI Blendstocks Have Minimal Impact on Cold-Start Emissions

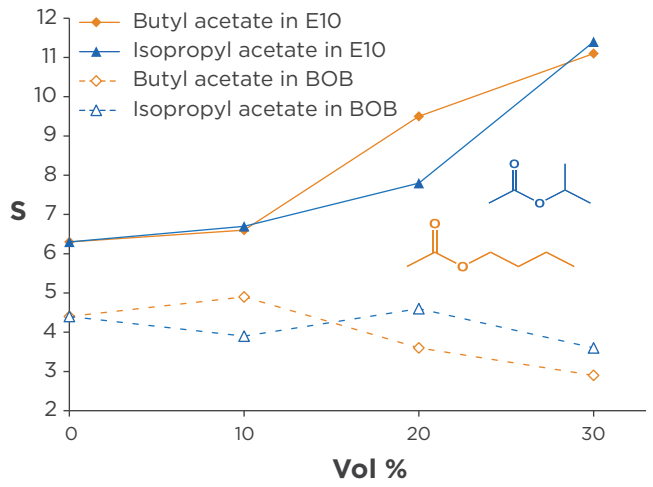
Advanced engines running on high-performance fuels must meet emissions regulations to be commercially viable. Because nearly all tailpipe emissions from boosted SI engines occur during cold start before the emissions-control catalysts are functional, fuel formulations that change catalyst light-off performance could impact emissions compliance. Researchers evaluated promising SI fuel blendstocks for catalytic light-off temperatures (the temperatures at which pollutants are converted to inert products) and determined that fuel chemistry significantly affected catalyst performance. However, when the blendstocks were blended into a surrogate fuel mixture (BOB) at concentrations of 10%–30%, they had minimal impact on catalyst light-off. The findings indicate that fuel blends containing up to 30% of these blendstocks will likely not have a significant impact on cold-start non-methane organic gas emissions from stoichiometric boosted SI engines.



Temperatures at which 50% (T50) and 90% (T90) of the Co-Optima blendstocks—ethanol, isobutanol, aromatic mix, and di-isobutylene—are converted over a three-way catalyst in a synthetic exhaust mixture containing 10%, 20%, and 30% blends in a surrogate BOB, and unblended (100%). Figure by Josh Pihl, ORNL

Unexpected Synergistic Blending Suggests Acetate Esters May Be Promising Blendstocks When Combined with Ethanol

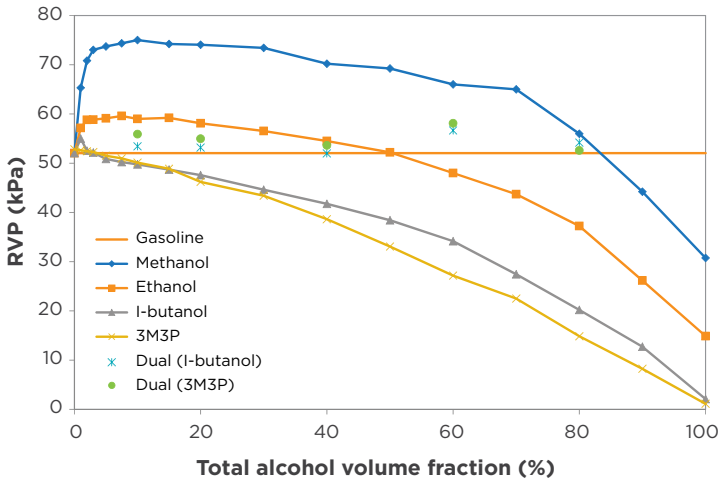
Acetate esters exhibit a very high RON when measured as pure compounds and, on this basis, could be considered promising boosted SI blendstocks. However, they blend antagonistically—enhancing performance less than expected based on linear blending assumptions using the pure component properties—for both RON and S when blended into a hydrocarbon base fuel. Because RON and S are critical to strong boosted SI engine performance, this antagonistic blending reduces the attractiveness of acetate esters as high-performance blendstocks. However, researchers discovered that adding 10% ethanol by volume and an acetate ester to a hydrocarbon fuel leads to synergistic blending, demonstrating more-than-linear increases in both RON and S when blended into the base fuel together, compared with blending the individual components. This result indicates that acetate esters may be promising blendstocks when used in conjunction with ethanol. The mechanism for this unexpected synergistic ester-ethanol blending is being investigated via detailed kinetics simulations to identify its underlying molecular basis and enhance understanding of how to optimize blending interactions among new bioblendstocks.



S vs. percentage of acetate ester blended (by volume) in BOB or E10. Blending esters in hydrocarbon BOBs does not increase S (dotted lines), while blending them in E10 does (solid lines). Figure by Evgueni Polikarpov, PNNL

Dual-Alcohol Gasoline Blends Overcome Single-Alcohol RVP Limitations

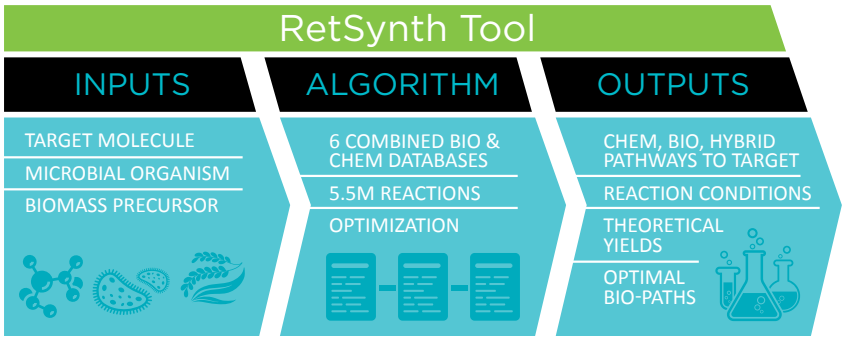
Co-Optima research has demonstrated the need to understand blending effects when creating fuels with properties that impart higher efficiency, such as high RON, S, and HOV. However, understanding blending effects related to other properties—including volatility and compatibility with fueling infrastructure—is also critical to ensuring that fuels meet commercial requirements. For example, co-blending ethanol/methanol and isobutanol/ethanol into a petroleum fuel mitigates the RVP increase of the lighter alcohol (methanol and ethanol, respectively). Researchers demonstrated that blending two alcohols with gasoline at up to 40% by volume can mitigate volatility issues associated with the lighter single-alcohol gasoline blends that have been the focus of much research to date. The researchers evaluated the azeotropic volatility behavior of single- and dual-alcohol gasoline blends by combining data from experimental monitoring of distillation composition evolution with results from a droplet-evaporation model. At all alcohol concentrations, properly designed dual-alcohol blends maintained RVP at levels very close to those of gasoline. These results suggest that higher alcohols such as isobutanol and 3-methyl-3-pentanol (3M3P) could be viable options for controlling RVP as dual blends in gasoline with lower alcohols.



RVP (in kilopascals [kPa]) vs. percentage of total alcohol (by volume) in gasoline for single-alcohol and dual-alcohol blends. Figure by Thomas Foust, NREL

RetSynth Tool Rapidly Identifies Viable, Optimized Production Pathways from Biomass to Biofuels

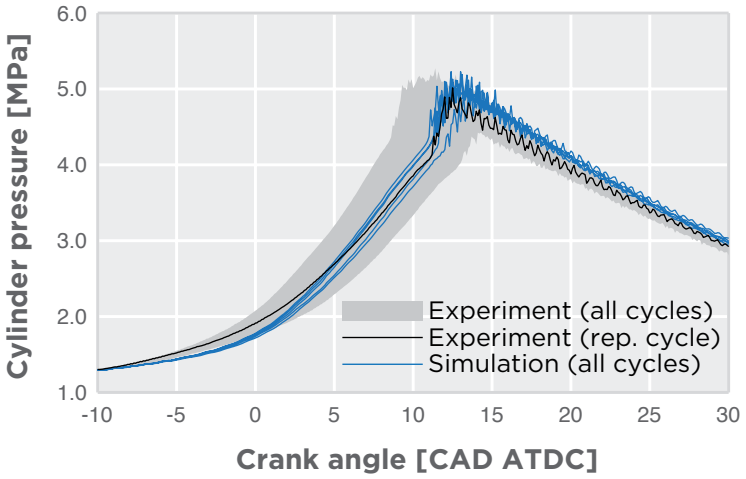
Researchers developed the RetSynth (retrosynthesis) tool to rapidly identify and evaluate the viability of pathways for producing bio-based molecules of interest to Co-Optima. Given a target molecule and a biomass-derived precursor and/or organism as input, RetSynth outputs the available biological, chemical, and hybrid production pathways. Included in the results are a list of genes, reaction conditions, and theoretical yields for the target molecule. For biological pathways, RetSynth can also rank the optimal routes with the smallest number of steps. In FY18, researchers demonstrated performance against existing retrosynthesis tools, showing RetSynth's ability to perform functions not present in other tools (i.e., bulk molecule assessment, chassis agnostic retrosynthesis, hybrid retrosynthesis) at efficiencies better than the state of the art. RetSynth was run for a large number of mixing-controlled compression ignition (MCCI), SI, and diesel-like compounds, including asymmetric ethers, methyl ketones, cyclopropenated fatty acid methyl esters (FAMEs), and 3,462 compounds not found in Escherichia coli K-12 MG1655 for potential synthetic routes to biological production. This tool is available at https://github.com/sandialabs/RetSynth.



Information flow of the RetSynth tool, which allows researchers to rapidly determine pathways of production to any target molecule. Figure by Anthe George, SNL, LBNL

Combustion Model Captures Multicomponent Fuel Composition Effects on Engine Knock

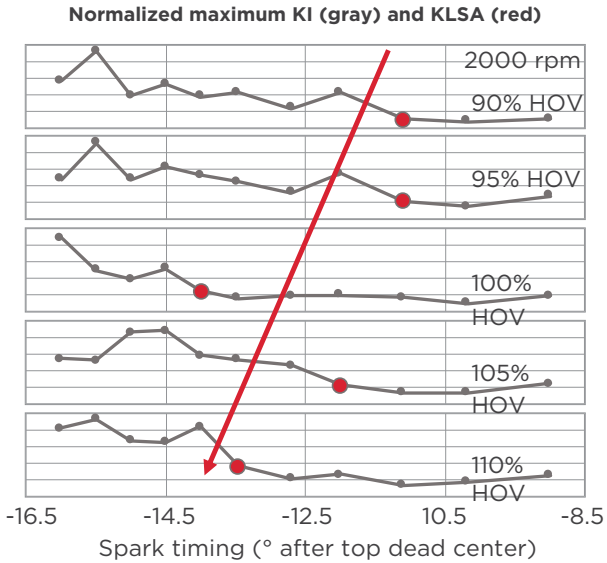
Knock is a major limitation to achieving higher thermal efficiency in SI engines. Knock prediction in computational fluid dynamics (CFD) simulations requires accurate descriptions of fuel autoignition and flame speed characteristics. Conventional SI combustion models base laminar flame speed on empirical correlations that are valid for only certain simple fuel blends and limited pressure-temperature-equivalence ratio ranges. Researchers developed an improved knock modeling framework that replaces conventional empirical correlations with a laminar flame speed lookup table generated a priori from a multicomponent chemical kinetic mechanism. When applied to a virtual CFR engine simulation tool, it captured combustion phasing, knock onset, and knock intensity (KI). This modeling approach accurately assesses the performance of complex multicomponent gasoline-biofuel blend surrogates under realistic engine operating conditions using CFD simulations. Current efforts are leveraging the novel virtual CFR engine model to investigate the impact of fuel composition and properties on engine efficiency under boosted SI and ACI conditions.



Validation of the virtual CFR engine model against experimental data for a knocking condition (fuel: iso-octane). ATDC = after top dead center; CAD = crank angle degree; MPa = megapascals; rep. = representative. Figure by Pinaki Pal, ANL

New CFD Approach Delivers Faster KLSA Prediction & Lower-Cost Global Sensitivity Analysis

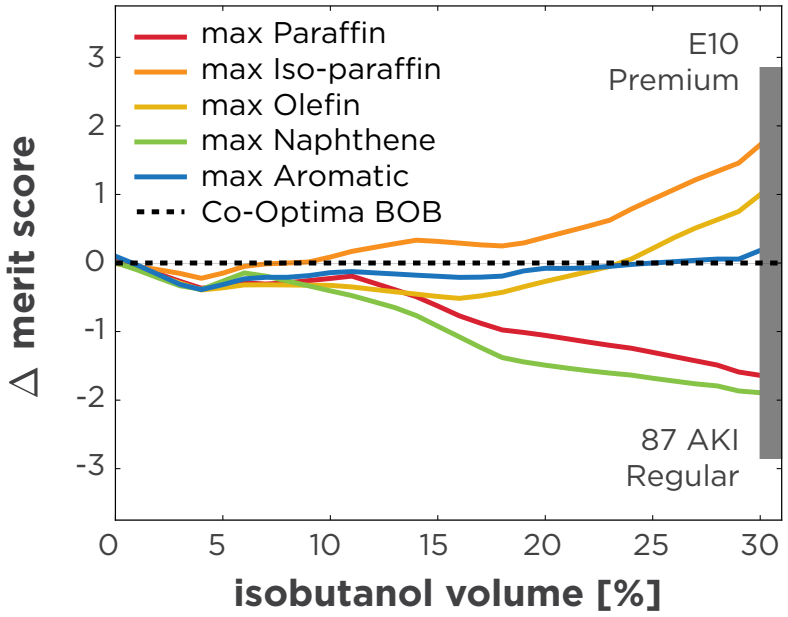
Knock-limited spark advance (KLSA) is defined as the spark timing at a given operating condition that provides the greatest engine torque. In practice it represents a compromise between SI engine efficiency and knock mitigation, and it depends on the knocking tendency of a fuel and engine condition. The use of CFD simulations to predict KLSA in SI engines is complicated by SI combustion's cycle-to-cycle variation and the need for a small time step (imposed by the numerical constraint of Mach Courant-Friedrichs-Lewy [CFL] number < 1). This gives rise to long simulation times to accurately capture in-cylinder pressure oscillations (equivalent to KI). Researchers developed a new method using multicycle engine simulations to account for cyclic variation, defining the KLSA as the slope change point in the maximum KI, which is insensitive to Mach CFL conditions. This approach allowed use of a large Mach CFL (50) for a run time at least three times faster. Simulation results on a stock boosted SI engine platform showed that KLSA changes along with HOV at a rate of -0.113 CAD per 1% HOV. This efficient CFD approach also enables global sensitivity analysis at reduced computational cost for independent identification of the impact of physical and chemical fuel properties that are difficult to investigate in experiments.



Normalized maximum KI as a function of spark timing for HOV values from 90% to 110% of baseline alkylate fuel. Each point is the maximum KI out of 10 consecutive-cycle simulations. Red dots are the predicted KLSA values. A linear fitting curve shows the HOV effect on KLSA is (-0.113CAD)/(%HOV) for alkylate at 2,000 rpm, 11.5 bar indicated mean effective pressure condition. Figure by Zongyu Yue, ANL

Virtual BOB Optimizations Show Importance of Synergistic Octane Blending

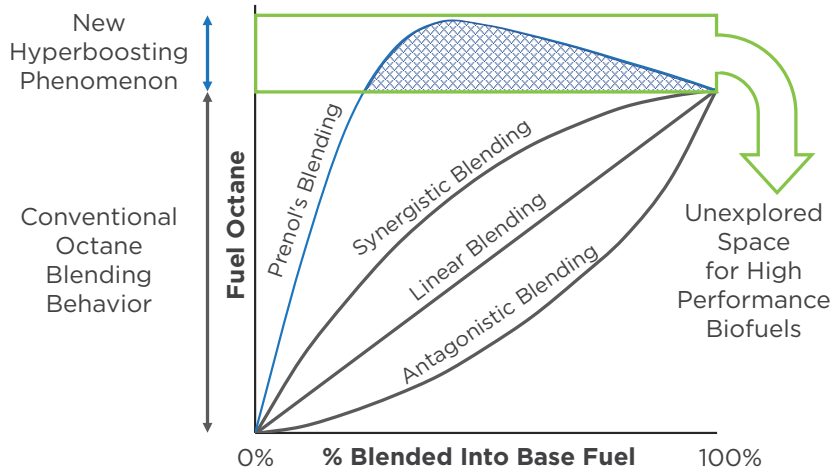
The opportunity for tailoring BOBs to exploit synergistic (better than linear) blending with a bio-derived blendstock was explored using a neural network octane predictor. Five virtual BOBs with widely varying compositions were created, with the same RON (90.3) and MON (84.7) as an experimentally tested Co-Optima BOB. The virtual BOBs were blended via simulation with 17 high-performance blendstocks at up to 30% by volume, and the potential to improve engine efficiency was measured by the change in the boosted SI merit function score. A one-point increase in the merit score indicated a potential improvement in engine efficiency of 1%. Nonlinear blending of the octane numbers led to synergistic and antagonistic (worse than linear) merit score gains depending on the composition of the BOB. For the five blendstocks with the largest blending variation in the virtual BOBs, the differences in merit function score due to nonlinear blending averaged 4%, corresponding to 60% of the benefit of switching from an 87 AKI finished fuel to one rated at 93 AKI. These results demonstrate the importance of matching a BOB and blendstock to maximize synergistic nonlinear blending effects. Successful experimental validation of this result will open the door for model-based fuel optimization, which could help fuel providers save money and energy designing a BOB for new blendstocks that minimizes octane giveaway.



Virtual BOB blending performance for isobutanol (solid lines) in terms of boosted SI merit score change from the four-component Co-Optima BOB (dashed line). Positive deviations represent merit function (efficiency) increases due to synergistic blending, while negative deviations represent decreases due to antagonistic blending. The results indicate that blending isobutanol in an iso-paraffinic BOB would yield much higher-performing fuels than if blended into a naphthenic BOB. The spread between the most synergistic and most antagonistic blends shown for isobutanol is more than 60% of the benefit of changing from 87 AKI gasoline to 93 AKI gasoline. Figure credit Matthew McNenly, LLNL

Discovery of Novel Octane Hyper-boosting Effect Suggests New Pathways to High-Performance Biofuels

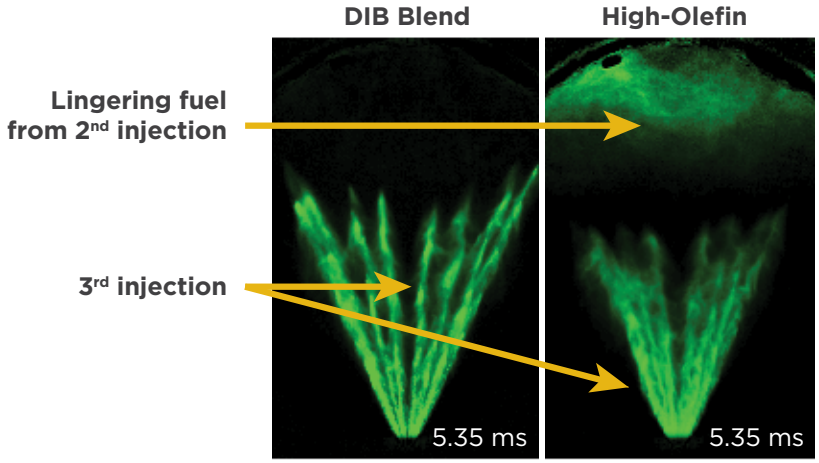
Co-Optima research has shown that blendstocks with beneficial properties for multimode engines—such as high RON, S, and HOV—alone are insufficient. They must also provide benefits in blends with petroleum BOBs. Ideally, a blendstock would provide nonlinear fuel-property improvements when combined with a BOB, and in fact candidates from some molecular families (e.g., alcohols, olefins) exhibit such synergistic octane blending. Researchers discovered, however, that fuel-property improvements even greater than observed with synergistic blending behavior are possible. When they blended prenol into different gasolines, the RONs of the resulting blends were higher than those of the prenol (93) or gasolines alone. This hyper-boosting phenomenon had not previously been observed when blending any other blendstock (oxygenate or hydrocarbon) into gasoline. The result is surprising, because a fuel's maximum RON is typically limited to the pure RONs of its individual components. Prenol's high blending RON and high S (19) may make it particularly suitable for high-efficiency multimode combustion approaches. Ongoing work is identifying the mechanism for prenol's blending behavior to determine whether this attribute may be exhibited by other blendstocks. If so, it could indicate other high-performance molecules that have been overlooked owing to relatively low pure blendstock RONs.



Schematic of fuel octane vs. percentage of blendstock blended into base fuel, showing prenol's hyper-boosting behavior pushing the blended fuel's RON beyond the level enabled by typical synergistic blending. Figure by Anthe George and Eric Monroe, SNL

Experiments Reveal Strong Fuel Effects on Sprays with Potential Impacts on Soot/PM Emissions

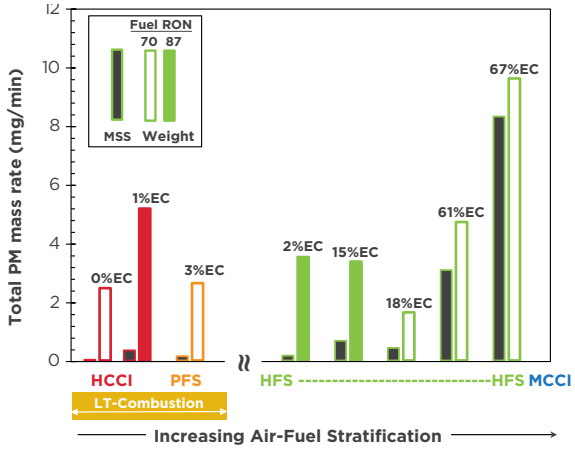
Co-Optima researchers recognized that accurate predictions of PM emissions under variable, real-world conditions must factor in fuel chemistry, fuel-air mixing characteristics, and engine operating conditions. Direct-injection SI engine experiments were conducted with nine fuels spanning wide ranges of PMI under several engine-operating strategies. Because the engine-out soot PM levels for a DIB blend and a high-olefin gasoline core fuel deviated strongly from expectations based on PMI, the spray formation for these fuels was examined in a constant-volume spray vessel with high-speed diffuse back-illumination. Counter to expectations based on its lower-temperature end-boiling point, the DIB-blend showed faster spray-tip penetration. Additionally, the high-olefin gasoline core fuel required significantly more time to complete vaporization. These findings highlight potential impacts of spray effects on the sooting tendencies of fuels and deficiencies of PMI for predicting engine-out PM.



High-speed diffuse back-illumination images of fuel injections in a constant-volume spray vessel, revealing that a DIB blend has longer spray-tip penetration compared with that of a high-olefin gasoline fuel, while the high-olefin fuel requires more time for complete vaporization. Images by Magnus Sjöberg and Scott Skeen, SNL

Air-Fuel Stratification Study Highlights Limitations of Established Methods for Measuring PM

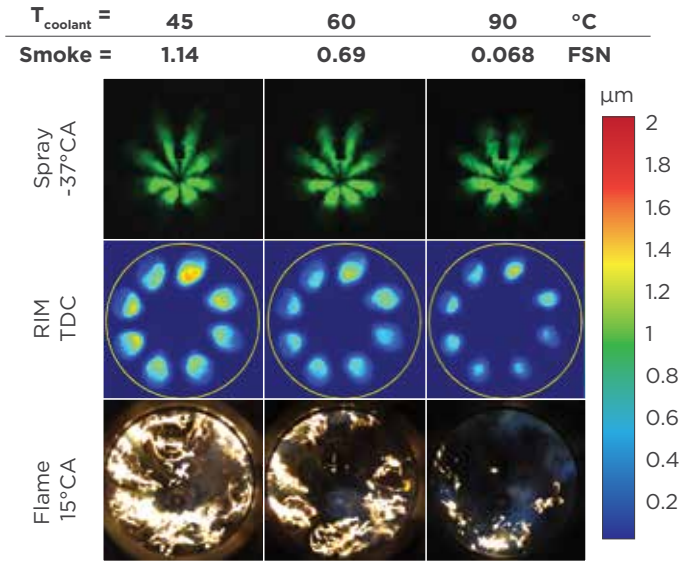
One key challenge to realizing commercial ACI engines is emissions control. Co-Optima researchers studied ACI operation in an LD engine over a range of air-fuel stratifications—from homogeneous charge compression ignition (HCCI) to a high fuel stratification (HFS) approach—to assess stratification impacts on PM formation. The researchers found that organic carbon (OC) dominates the PM mass over most of the stratification range. Elemental carbon (EC) was not a significant contributor to the PM mass until almost complete air-fuel stratification had been reached. For similar ACI approaches and air-fuel stratification levels, the RON 87 fuel generated greater levels of PM mass compared with the RON 70 fuel. However, it is still unclear if the increase was related to a chemical or physical fuel property effect. Measurements also revealed that the widely used AVL Micro Soot Sensor (MSS) failed to capture as much as 90% of the PM mass collected by sample filters, used in regulatory compliance measurements, with the discrepancies being greatest as the fraction of OC in the PM increased. The inability of the MSS to measure OC-based PM mass characteristics of ACI emissions indicates that PM mass measurements beyond the MSS should be included when reporting PM production under ACI modes.



PM mass emissions rates for ACI modes using gasoline-range fuels (RON 70 and 87) including HCCI (red), PFS (partial fuel stratification, orange), and HFS (green). MCCI (blue) is included in the graph, but no data were collected. Black bars indicate the soot mass emissions rates from MSS data. Colored bars are from gravimetric filter measurements (empty = RON 70 fuel; solid = RON 87). The %EC listed indicates the fraction that was EC, with the remainder being OC. Engine: 1.9-L diesel platform. Combustion timing, speed, and torque (2,000 rpm and 4/5 bar brake mean effective pressure) were kept constant for each fuel. LT = low-temperature. Figure by Melanie DeBusk, ORNL

Increased Cold-start Smoke Emissions Linked to Stratified SI Engines Using E30 Fuel

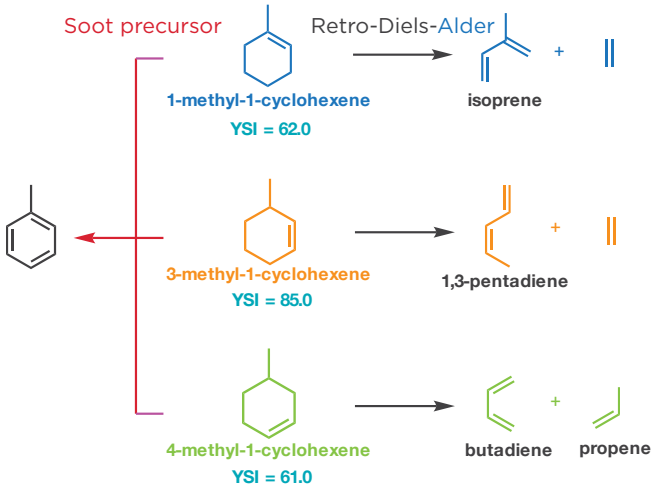
Advanced lean stratified-charge SI engine operation can offer high thermal efficiency for multimode approaches, but can also increase PM emissions. Any new alternative gasoline fuel formulations will need to be assessed for compatibility with advanced combustion modes, including cooler engine operating conditions encountered during cold start and engine warm-up phases. Researchers showed that use of E30 (gasoline blended with 30% ethanol) can lead to unacceptably high levels of smoke emissions for operation at low coolant temperatures under lean stratified-charge SI conditions. Using an optical refractive index matching (RIM) technique to measure fuel film on the engine piston top resulting from the fuel sprays wetting the wall, researchers discovered that lower coolant temperatures greatly increase fuel film area and thickness, resulting in more soot-generating pool fires and exhaust smoke emissions. These findings reinforce the importance of identifying and addressing how changes in gasoline composition might affect combustion systems, to avoid issues when introducing new fuels to market.



Effect of engine coolant temperature on fuel sprays (top), piston-top fuel films (middle), and flames (bottom). Scale at right relates to the thickness of the piston-top fuel films. TDC = top dead center; CA = crank angle; FSN = filter smoke number, a measure of soot emissions. Figure by Magnus Sjöberg (SNL) and Xu He (Beijing Institute of Technology)

Researchers Identify New Soot Formation Chemistry Impacting Emissions from Direct-Injection SI Engines

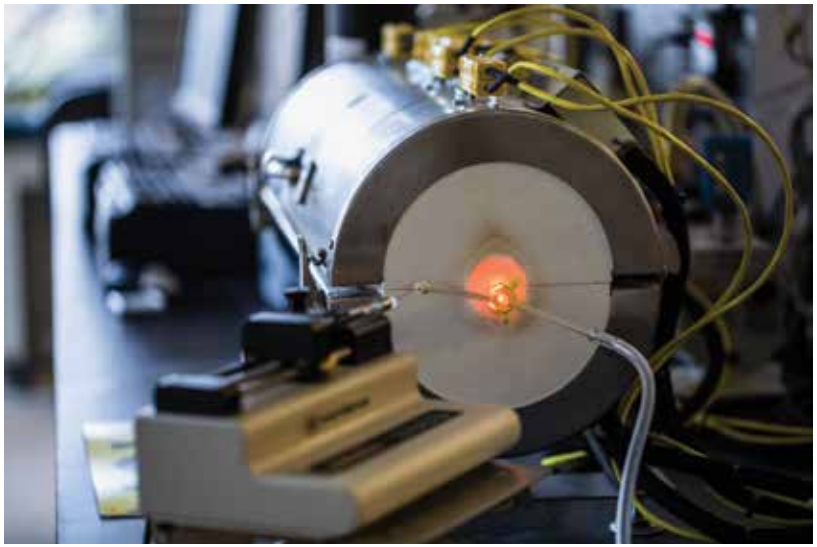
Gasoline combustion in direct-injection SI engines can produce significant fine particle emissions (soot). Yet, the ways in which gasoline components react to form soot precursors and, ultimately, fine particles are poorly understood. Measurements of yield sooting index (YSI) for three methylcyclohexene isomers (representative components of commercial gasolines) indicate there is new or unusual reaction chemistry not captured in a recent model for molecular-structure effects on soot formation. Researchers performed a combined flow reactor experimental and theoretical study to clarify the drivers of soot formation. The researchers demonstrated that 1-methyl-1-cyclohexene and 4-methyl-1-cyclohexene preferentially react via a ring opening and molecular weight reduction—pathways that do not lead to accelerated soot formation. However, 3-methyl-1-cyclohexene, which produces much more soot in experiments, preferentially reacts via dehydrogenation to cyclic dienes—a pathway leading to aromatic ring formation and fine particles. Quantum chemical calculations confirmed the kinetic basis for enhanced soot formation of 3-methyl-1-cyclohexene and contributed to updated kinetic models for the three isomers. These results demonstrate that the relative stability of the first radical intermediate determines the branching ratio between formation of soot precursors and ring-breaking retro-Diels-Alder reaction products.



Reactions of three methylcyclohexene isomers to produce toluene as a soot precursor and newly identified retro-Diels-Alder reaction products via ring-opening reactions that do not lead to soot formation. Figure by Seonah Kim, NREL

Flow Reactor Research Reveals Autoignition & Soot-Precursor Formation Chemistry of High-Octane Blendstocks

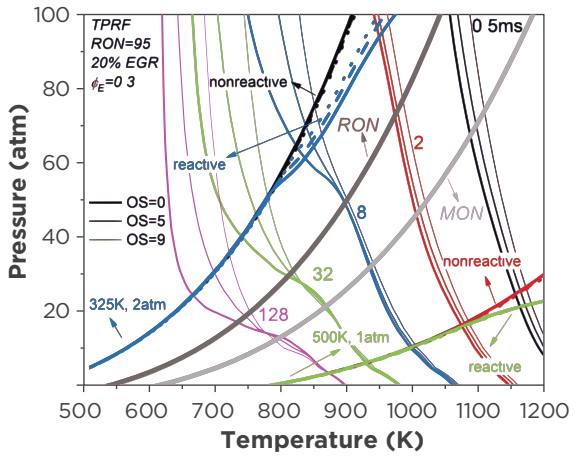
An accurate understanding of kinetic mechanisms can indicate how molecular structure impacts fuel properties. Researchers used flow reactor studies to improve understanding of the kinetics of autoignition and soot formation while informing the development of kinetic simulation tools. Flow reactor studies of fuel autoignition chemistry were carried out over a wide temperature range for ethanol, n-propanol, i-propanol, i-butanol, anisole, cyclopentanone, DIB, and dimethyl furan. Results were compared with simulations from the Co-Optima kinetic model. Although the kinetic model predicted reactant conversion and the formation of one- and two-carbon products well, there was poor agreement for other intermediate species. These results have been used to develop an improved kinetic model for these important blendstocks. In another related study, the results of flow reactor experiments were used to help identify the different reaction pathways of the three positional isomers of methylcyclohexenes that were not captured by the model based on molecular structure. Collectively these results demonstrate the utility of species-resolved flow reactor experiments in elucidating the fundamental steps of key autoignition and soot formation processes.



Laminar flow reactor and analytical system. Photo by Werner Slocum, NREL

Autoignition Analysis Informs Prediction of Fuel Performance Under ACI Conditions

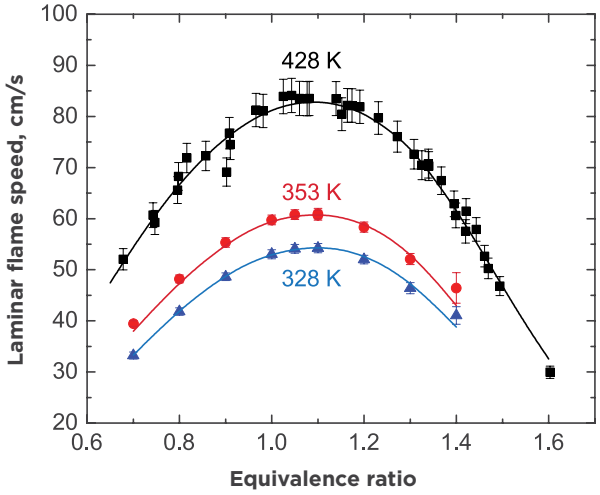
Researchers analyzed autoignition under a wide range of engine conditions to improve predictions of fuel performance in ACI engines. Earlier work suggested that metrics for predicting performance under traditional SI conditions—including RON, MON, and S—may be inadequate for predicting performance under ACI conditions. For this reason, the researchers explored the entire range of SI and ACI engine conditions by overlaying modeled engine pressure-temperature trajectories onto modeled fuel ignition-delay contours. In the analysis pictured in the figure, for example, the autoignition impact of S was small (closely spaced ignition-delay contours) at high temperatures and low pressures, but large (widely spaced ignition-delay contours) at low temperatures and high pressures; to predict performance accurately, the weighting of S would need to vary according to ACI pressure-temperature regimes. This approach clarifies the chemistry- and condition-dependent impacts of numerous factors needed to predict fuel performance under SI and ACI conditions.



Example pressure vs. temperature plot showing autoignition analysis: engine thermodynamic trajectories (rising from left to right) overlaid onto ignition-delay contours for toluene primary reference fuel (TPRF) with three different S (falling from left to right, labeled with delay in milliseconds). EGR = exhaust gas recirculation, φE = actual fuel/air ratio divided by stoichiometric fuel/air ratio. Figure by Peng Zhao, Oakland University, and Patrick Lynch, University of Illinois at Chicago

Molecular Basis of Cyclopentanone's High Flame Speeds Identified Via Combined Experimental & Modeling Study

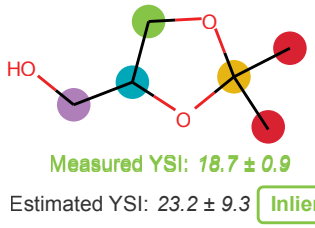
Fuels with higher laminar flame speeds have been shown to increase SI engine efficiency, particularly under highly lean and/or dilute conditions. Cyclopentanone has been identified as a high-performance blendstock based on its high RON (101), high S (11), and good blending characteristics. It also has been shown to have high laminar flame speeds. Because of these beneficial attributes, researchers simulated cyclopentanone flame speeds using a kinetic model developed via high-level chemistry calculations, and they compared predictions against fundamental experimental data on laminar flame speeds, carbon monoxide time histories, and ignition-delay times for the model validation and optimization. The kinetic model accurately predicted the reactivity of cyclopentanone over a wide range of conditions. The newly validated model allows reliable prediction of flame speeds under engine pressures and temperatures. It shows that cyclopentanone's high flame speed is due to high yields of ethylene that subsequently produce reactive vinyl radicals. Kinetic models for cyclopentanone and other high-performance fuels are critical to enabling multidimensional engine simulations that help co-optimize efficiency and performance when these fuels are used in engines with advanced combustion modes.



Predicted (curves) and measured (symbols) laminar flame speeds of cyclopentanone at different equivalence ratios (actual fuel/air ratios divided by stoichiometric fuel/air ratios) and unburned gas temperatures. Figure by Kuiwen Zhang, LLNL

Interactive YSI Tool Accelerates Estimation of Blendstock Sooting Tendency

Although LD gasoline engines generally operate with low soot emissions, some operating conditions being explored for advanced LD engines have been shown to increase PM levels. Consequently, it is important to characterize the sooting and PM formation behavior of promising new blendstocks. Researchers integrated the YSI computational method into a tool that rapidly estimates the sooting tendency of fuel blendstocks, allowing the interactive development of potential new blendstocks that meet YSI targets. Experimental data on sooting tendency are continually added to the YSI database to broaden the scope of the compounds analyzed and improve prediction accuracy, which has enabled the tool to provide estimates across multiple orders of magnitude of sooting tendency. The tool's detailed accounting of the data that lead to a given prediction allows users to determine if the prediction for an unmeasured compound is reasonable. In addition, collaborative tool development has facilitated frequent updates with YSIs of newly synthesized experimental compounds, furthering the use of YSI as a metric for designing low-sooting fuel surrogates. The tool is available at https://ysipred.herokuapp.com.



Component Fragments

[H]-[C](-[H])(-[H])-[C]
Count: 2
YSI: 9.1 ± 8.0
Training #: 786

[C]-[C](-[C])(-[O])-[O] | (Ring)
Count: 1
YSI: 10.5 ± 10.3
Training #: 4

[H]-[C](-[H])(-[C])-[O] | (Ring)
Count: 1
YSI: 12.5 ± 8.3
Training #: 17

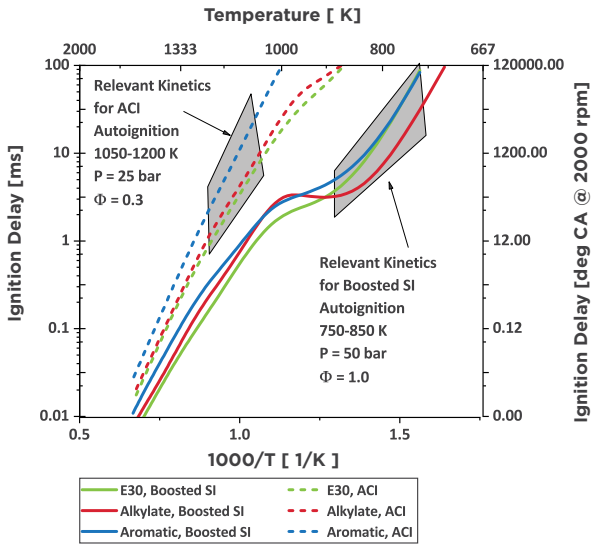
[H]-[C](-[C])(-[C])-[O] | (Ring)
Count: 1
YSI: 19.1 ± 8.8
Training #: 14

[H]-[C](-[H])(-[C])-[O]
Count: 1
YSI: 10.4 ± 8.0
Training #: 117

Screen capture of YSI estimation tool, detailing the data used to generate the YSI prediction for the target molecule. Figure by Peter St. John, NREL

Kinetic Modeling Suggests the Need to Improve Fuel-Quality Metrics for SI/ACI Multimode Combustion

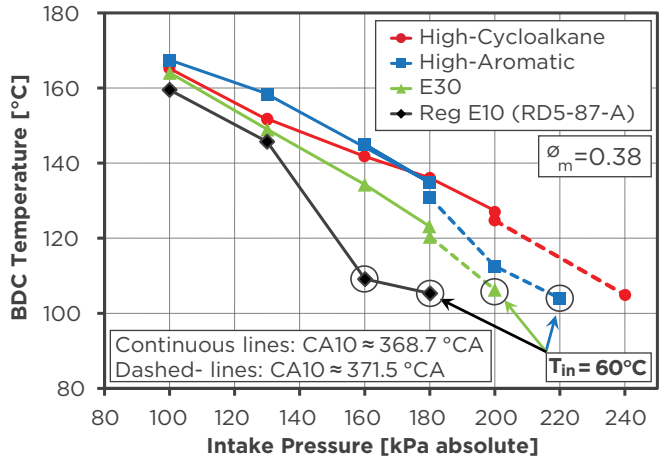
Determining fuel characteristics that enable efficient operation under multiple operating regimes is critical to advancing multimode engine technologies. Researchers used kinetic modeling to explore the predictive capability of OI across various fuel types and engine operating conditions. OI has been used to quantify a fuel's resistance to autoignition at elevated pressures, but its ability to predict the performance of gasoline-based fuels during ACI operation has been uncertain. Three Co-Optima gasoline-range core fuels with matched RON and different compositions were investigated: high aromatic, high alkylate, and E30. If OI is a valid predictor of fuel combustion under ACI conditions, each fuel should show ignition delays that correlate with its RON and MON. This was the behavior predicted by the model under boosted SI conditions, where the aromatic and E30 fuels (which have RON 98 and MON 87–88) ignited later than the alkylate fuel (RON 98, MON 97), confirming the experimental observation that OI is a good predictor of boosted SI ignition. However, under ACI conditions, the aromatic fuel and E30 ignition delays did not match, which is inconsistent with OI expectations. Instead, the aromatic fuel was the least reactive, and the E30 was the most reactive. The results indicate that a chemistry-specific effect not captured by OI is driving performance under these ACI conditions, and that new metrics are warranted.



Kinetic modeling results: fuel reactivity (ignition delay) vs. temperature, with shaded regions representing temperature ranges important for autoignition, for boosted SI operating conditions and ACI operating conditions. Φ = actual fuel/air ratio divided by stoichiometric fuel/air ratio; deg CA = degrees CA; T = temperature. Figure by Jim Szybist, ORNL

Predictive Shortcomings of RON & MON Surface in High-Boost Engine Experiments

Researchers provided additional evidence that new reactivity metrics are required to specify fuels for high-efficiency, dilute combustion regimes relying on compression ignition. Three fuels with different compositions—high-cycloalkane, high-aromatic, and E30—but the same RON (98) and MON (87) had widely varying autoignition reactivities under dilute conditions, indicating that RON, MON, and the OI (deduced from RON and MON) fall short in characterizing their autoignition behavior. Findings also suggest that blending of cyclopentane (the primary cycloalkane in the high-cycloalkane fuel) could benefit future boosted SI fuels owing to the fuel's low reactivity at high-boost pressure. The high-cycloalkane fuel exhibited autoignition reactivity between that of the high-aromatic and E30 fuels at lower intake pressures, while showing the least reactivity of all fuels at intake pressures greater than 1.8 bar. E30 was the most reactive fuel at all intake pressures tested. These results, combined with identification of deficiencies in existing ignition metrics for ACI combustion, provide the insight needed to more precisely define ignition metrics and predict ACI combustion performance.



Bottom dead center (BDC) temperature required to achieve autoignition (CA10) at the specified CAs in a homogeneous fuel-air mixture for three gasoline blends (RON 98, MON 87) and regular E10 (RON 92, MON 85). The required BDC temperature is a measure of the fuel's autoignition reactivity, with higher temperatures corresponding to less reactive fuels. Φm = mass-based equivalence ratio, a measure of the fuel/air ratio. Figure by John Dec, SNL

> Medium- & Heavy-Duty Vehicle Research

Medium-duty (MD) and heavy-duty (HD) vehicles present operational and efficiency challenges that are distinct from those of light-duty vehicles. Co-Optima MD and HD vehicle projects are investigating approaches that range from mixing-controlled compression ignition (MCCI) to advanced compression ignition (ACI) concepts.

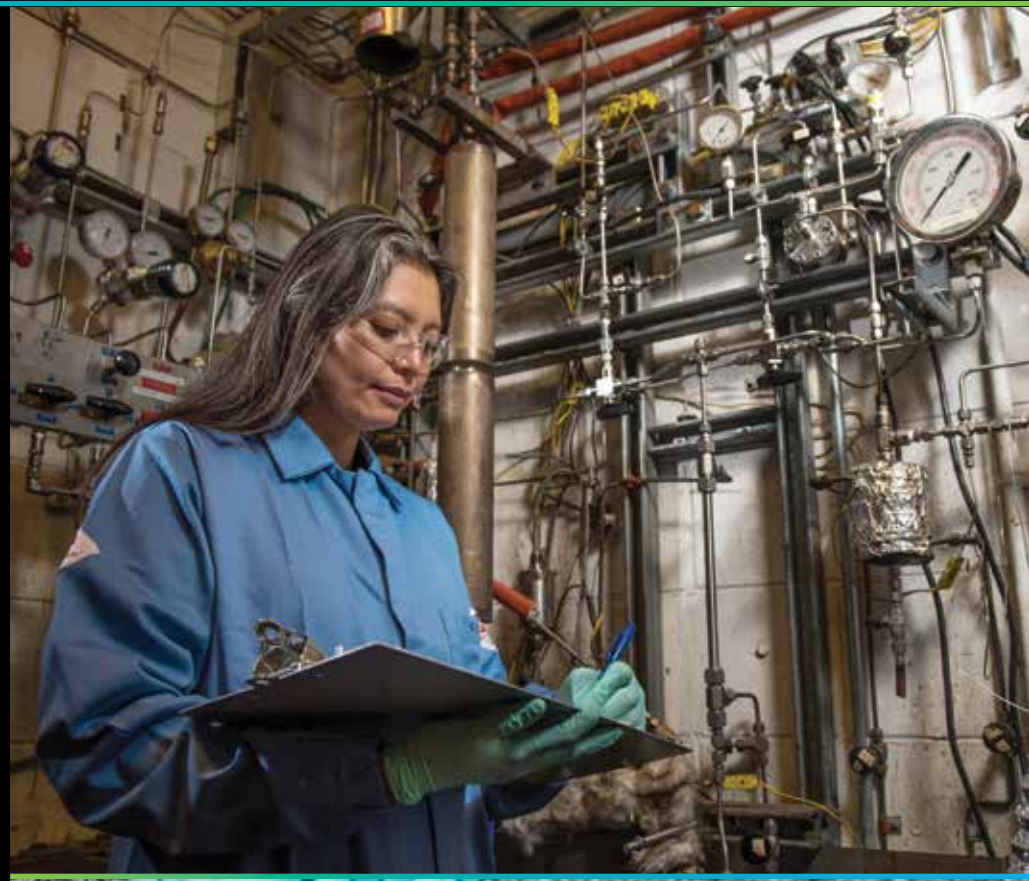
Co-Optima MD/HD Vehicle Targets

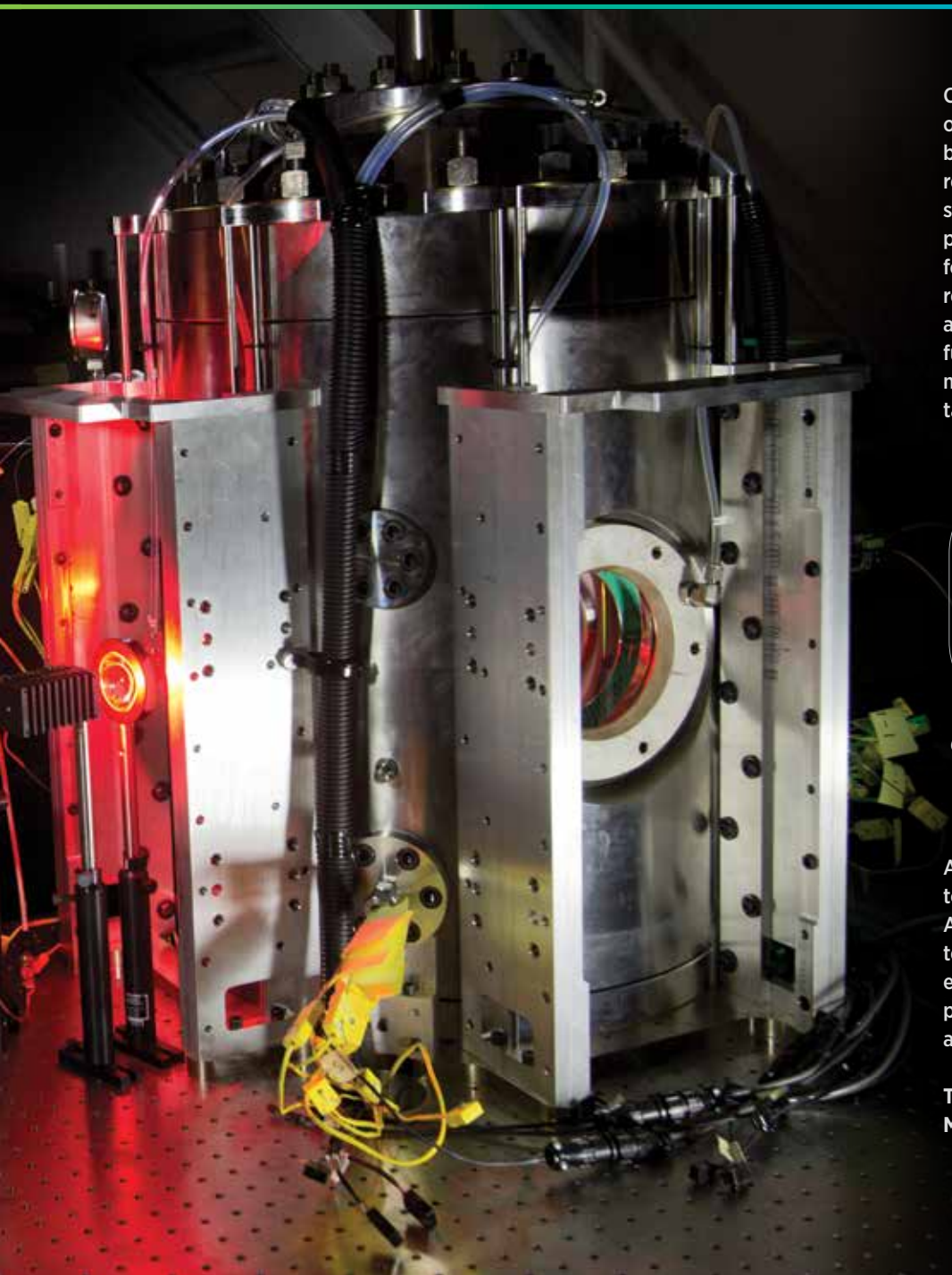
60% ENGINE BRAKE THERMAL EFFICIENCY

50% REDUCTION
PARTICULATE MATTER (PM)
NITROGEN OXIDES (NO_x)
HYDROCARBON (HC)
CARBON MONOXIDE (CO)

Today's MCCI diesel engines are extremely efficient, but they require complex and costly emissions-control technologies. Co-Optima MCCI research is working to maintain or improve MD and HD engine efficiency and fuel energy density while making compliance with the next tier of criteria emissions regulations more affordable. The MCCI research portfolio also includes a longer-term effort examining ducted fuel injection, a novel combustion technology that may significantly decrease in-cylinder soot production while maintaining high efficiency.

Fiscal Year 2018 (FY18) MCCI blendstock identification and evaluation activities explored a spectrum of chemical functional groups and production routes. Targeted screening of potential MCCI blendstocks from 18 chemical families assessed physical properties, cetane numbers, cold-flow properties, energy densities, and abilities to reduce particulate matter (PM).





Co-Optima researchers completed a systematic assessment of the suitability of hydrocarbon and oxygenate functional groups—all potentially derived from biomass and representative of a diverse range of structures and chemical reactivity—for use as diesel-like blendstocks in an advanced MCCI engine. Results show that alkanes, cyclic alkanes, alkenes, ethers, polyethers, and esters are promising candidates for MCCI blendstocks due to properties including low soot-formation, high cetane number, good cold flow, and established diesel distillation requirements. These findings combined with techno-economic (TEA) and life cycle analyses (LCA) point to blendstocks that, when blended with petroleum-based fuels, are likely to reduce PM emissions and maintain high efficiency, as well as meet fuel economy, cost, environmental performance, and other fundamental targets.

MCCI Blendstock Screening Results

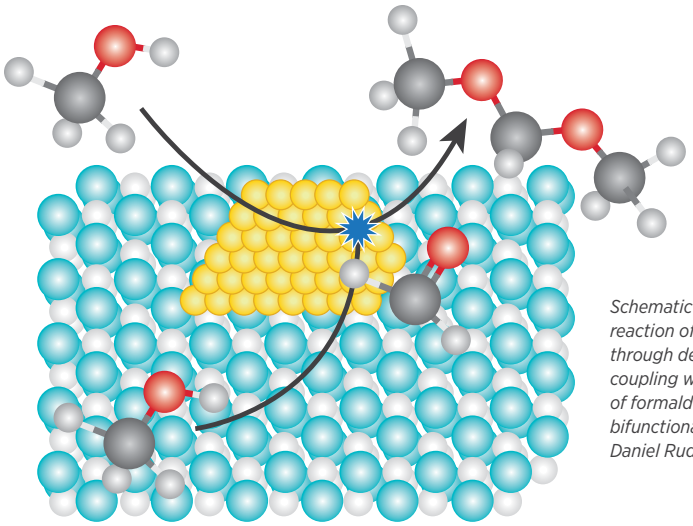
Compounds from a wide variety of chemical familes have been evaluated for suitability as MCCI blendstocks. Six families have been identified that are able to broadly meet performance targets, while seven others may include suitable candidates.

ACI combustion is a potentially transformative technology that has the potential to simultaneously deliver high thermodynamic efficiencies and low emissions. Although Co-Optima MD/HD ACI combustion research is at an early stage, the team has begun tackling significant scientific and engineering challenges, examining fuel properties and engine parameters needed for optimal efficiency, power density, and wide operability, as well as effective emissions control and aftertreatment strategies.

The following highlights provide more detail on FY18 accomplishments related to MD and HD vehicles.

Synthesis of Oxymethylene Ethers from Methanol Suggests a Path to Cost-Effective New Diesel Blendstocks

A key goal of Co-Optima medium-duty (MD) and heavy-duty (HD) vehicle research and development (R&D) is identification of diesel-boiling-range blendstocks that reduce PM emissions and can be readily derived from biomass. Researchers took a step toward demonstrating the cost-effective conversion of bio-derived methanol to poly (oxymethylene) ethers (OMEs), which hold potential for reducing soot emissions and increasing cetane number in diesel fuels. The new method circumvents the formaldehyde isolation required in traditional conversion routes by combining methanol dehydrogenation to formaldehyde with coupling to OME products in a single reactor. A promising copper-zirconia-alumina ($Cu/ZrOx\text{-}Al_2O_3$) catalyst developed for this one-step reaction demonstrated increased conversion of methanol to OME products by 16%—surpassing a stretch target of 10%—and increased methylal selectivity by 25% versus the baseline reaction using a molybdenum-carbide catalyst. Ongoing research will further develop the improved catalyst and process to extend the dehydrogenative coupling chemistry to higher alcohols (e.g., ethanol and butanol).

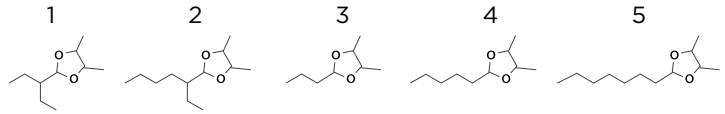


Schematic of the one-step reaction of methanol to OMEs through dehydrogenative coupling with in-situ generation of formaldehyde over a bifunctional catalyst. Figure by Daniel Ruddy, NREL

Ethanol-Based Diesel Blendstocks Offer Potential Cost, Performance & Emissions Benefits

Researchers developed a novel pathway for converting ethanol and 2,3-butanediol (BDO) to 1,3-dioxolanes—diesel-boiling-range bioblendstocks that offer potential cost, performance, and emissions benefits. The process operates below 40°C, captures 95% or more of the reactants' carbon, and results in phase separation that enables easy product recovery. The commercially available catalyst used in the reaction exhibits no degradation after 10 reaction iterations. These characteristics suggest this process could be cost-effective at scale. In addition, the low viscosities and freezing points of the five 1,3-dioxolanes produced may make them promising blendstocks for cold-weather fuels. Although the new blendstocks' energy densities average about 20% lower than diesel's, their soot-forming tendencies are significantly lower. Four products also have similar or better cetane numbers than those of diesel. These bioblendstocks present opportunities to increase and diversify ethanol use while enhancing the performance and emissions of compression-ignition engines powered by renewable fuel blends.

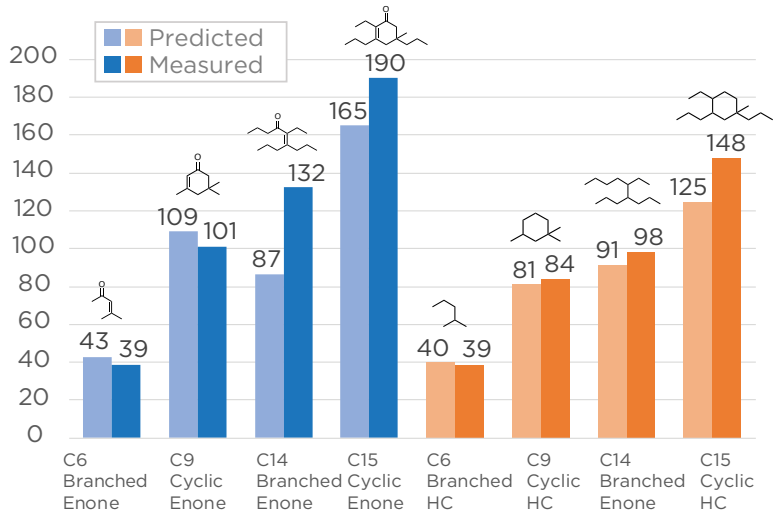
Compound	LHV ($MJ\ kg^{-1}$)	YSI	F.P. (°C)	B.P. (°C)	Viscosity (40 °C, $mm^2\ s^{-1}$)	DCN
1	32.98	57.8	< 100	174	1.26	44.8
2	34.36	68.5	< 100	184	1.88	64.2
3	30.95	36.5	< 100	161	0.94	33.4
4	32.92	48.7	< 100	177	1.49	48.1
5	34.04	63.2	< 100	188	2.34	68.9
Co-Optima Tier 1 Screen	> 25.00	Diesel 220	< 0	< 338	---	> 40



Molecular structure and summary of fuel properties for five 1,3-dioxolane compounds. DCN = derived cetane number, LHV = lower heating value (energy density), YSI = yield sooting index (measure of soot emissions from combustion), F.P. = freezing point, B.P. = boiling point. Figures and table by Andrew Sutton, LANL

Coupling Fermentation-Derived Mixed Acids Forms Promising MCCI Bioblendstocks

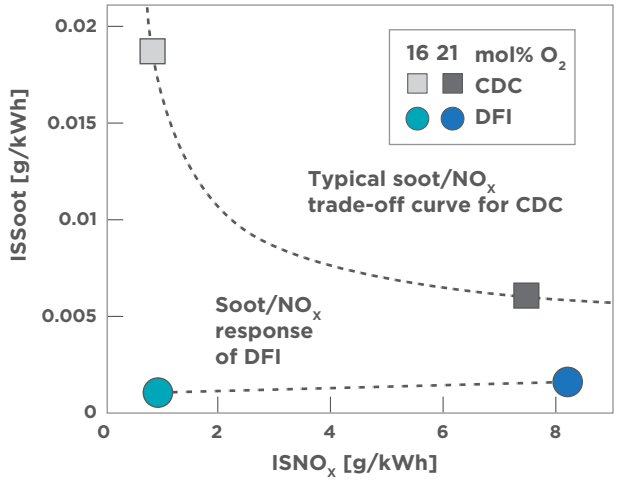
Bioblendstocks with desirable properties for MCCI engines—such as high cetane number (CN), low-yield sooting index (YSI), and good cold-flow properties—could provide high-value options to producers of future HD vehicle fuels. Researchers systematically screened potential MCCI fuels that can be produced by coupling mixed acids generated by fermentation to form coupled enones. CN and YSI were modeled to identify the most promising structures for enones as well as their hydrocarbon (HC) analogues produced via hydrotreating. Small quantities of select compounds were synthesized for experimental evaluation. The experiments provided data to improve the predictive YSI models for enones. Experimental results confirmed that enones consistently display a higher sooting tendency, suggesting that the HCs are the more promising MCCI blendstocks, and that the additional hydrotreating step in this chemical pathway is beneficial.



Predicted YSI from the new model and measured YSI for four enone compounds and their HC analogues, showing lower soot emissions from the HCs. Figure by Derek Vardon, Peter St. John, and Seonah Kim (NREL); and Charles McEnally (Yale University)

Ducted Fuel Injection Dramatically Decreases Diesel Soot Emissions

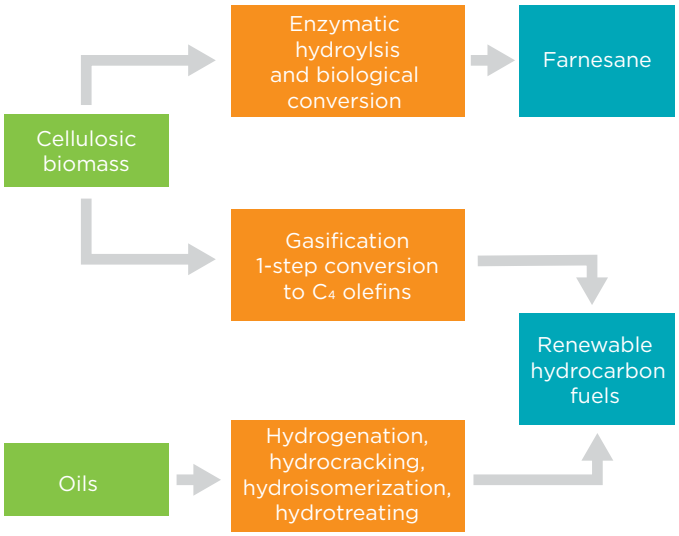
Ducted fuel injection (DFI) is a new concept for enhancing fuel-air mixing in MCCI engines by directing fuel sprays into small, co-axial ducts aligned with the spray axes. The first-ever DFI experiments in an engine indicated that DFI with moderate intake dilution can significantly decrease the soot emissions typically generated by diesel combustion, while maintaining comparable nitrogen oxide (NO_x) emissions. Compared to conventional MCCI at the same dilution, DFI produced soot emissions approximately an order of magnitude lower, while preserving simple control of ignition timing. When combined with intake-mixture dilution (16 mol% O_2 in the figure), DFI simultaneously curtailed soot and NO_x emissions. While these initial results were obtained using a commercial diesel fuel, experiments in FY19 will examine whether DFI performance can be further enhanced by fuel composition and properties.



Comparison of indicated-specific (IS) engine-out emissions of soot and NO_x for conventional diesel combustion (CDC) vs. DFI, as a function of intake-mixture dilution (i.e., oxygen mole fraction, mol% O_2). Figure by C.J. Mueller, SNL

Screening Concludes Assessment of Bioblendstocks for Heavy-duty Engines

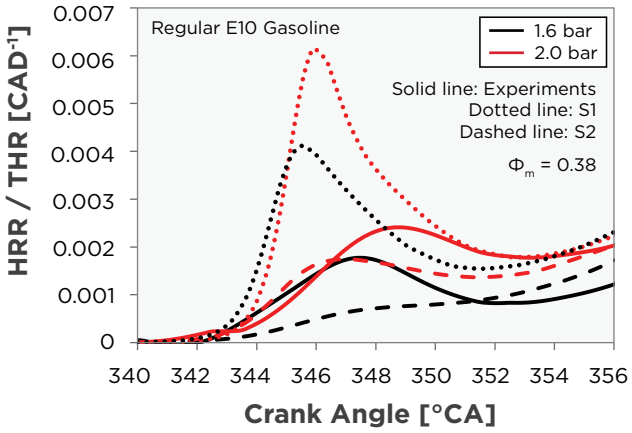
In FY18, the Co-Optima team began analyzing the economic, scalability, and sustainability feasibility of bioblendstocks for use in MD and HD engines, with an initial focus on MCCI engines. As a preliminary step, researchers evaluated farnesane, an emerging bioblendstock, and two benchmark renewable diesels—both hydrocarbon mixtures in the diesel boiling range—produced via two different pathways. These blendstocks were evaluated against 18 criteria characterizing technology readiness, economic viability, and environmental impacts. The evaluation concluded that, in general, the three bioblendstocks exhibited favorable scalability, technology readiness, and environmental characteristics. Continued holistic evaluation of economic factors and environmental effects, including water consumption, will be critical to guiding Co-Optima research efforts.



Pathways for bioblendstocks for heavy-duty engines. Figure by Jennifer Dunn, ANL

New Method for Developing Fuel Surrogates via Fuel-Composition Analysis Improves Engine Modeling

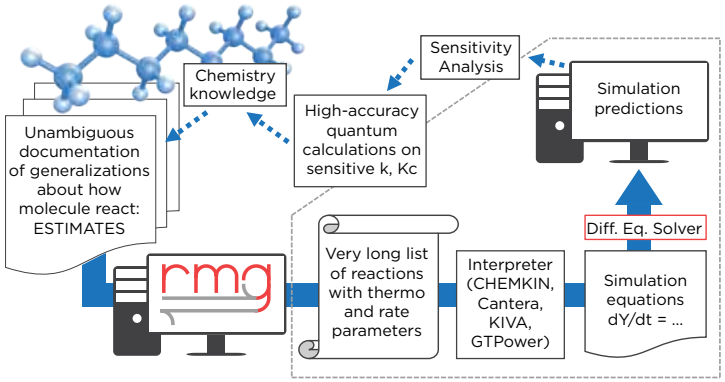
The inordinate computational resources required to model the combustion behavior of complex fuels like gasoline have led researchers to use simplified fuel surrogates in high-fidelity engine simulations. However, a previously available surrogate (S1) for regular E10 (gasoline containing 10% ethanol)—which had been developed through the accepted method of matching research and motor octane numbers (RON and MON) and agrees well with conventional spark ignition engine data—predicted autoignition occurring much too early under turbocharged conditions in a homogeneous charge compression ignition (HCCI) engine. To mitigate this issue, researchers developed a new gasoline surrogate (S2) by matching molecular types and sizes from detailed hydrocarbon analyses of the real fuel, rather than matching RON and MON. Compared to the S1 results, the simulated S2 results much more closely matched combustion experimental results, as well as the RON and MON of the gasoline of interest. The researchers developed new surrogates for high-cycloalkane, high-aromatic, and E30 (gasoline containing 30% ethanol) core fuels using this new methodology. Compared with the previous surrogates, all three new surrogates much more closely matched experimental results under both naturally aspirated and boosted conditions.



Early low-temperature heat release rate (HRR) normalized by the total heat release (THR) versus crank angle for a regular E10 gasoline in an HCCI engine at absolute intake pressures of 1.6 bar (black) and 2.0 bar (red). Modeling results for the previously available S1 surrogate (dotted lines) and the new S2 surrogate (dashed lines) are compared with experimental measurements (solid lines). Top dead center is at 360°CA. Φ_m = actual fuel/charge-mass ratio divided by stoichiometric fuel/air ratio. Figure by John Dec, SNL

Automated Chemical Mechanism Generator Saves Time & Cost by Rapidly Constructing Biofuel Models

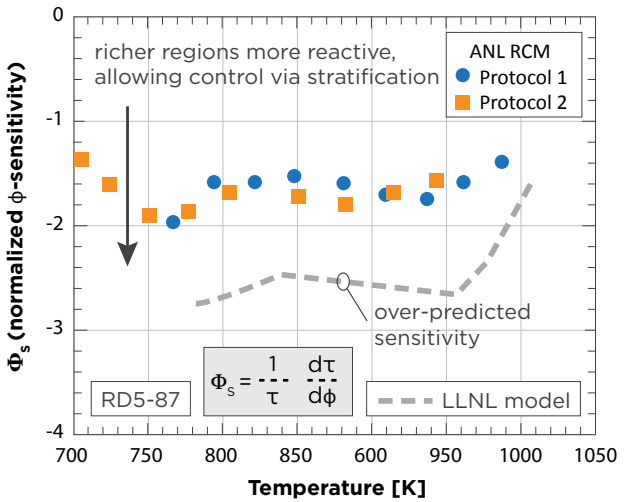
Detailed chemical kinetic mechanisms are essential elements of numerical combustion simulations, and accurate mechanisms are critical for reproducing important phenomena such as combustion timing and emissions. Researchers demonstrated the utility of the Reaction Mechanism Generator (RMG) software in developing and validating a chemical kinetic model for combustion of methyl-propyl ether (MPE), a promising class of diesel boiling-range bioblendstock candidates. The RMG constructs kinetic models composed of elementary chemical reaction steps using a general understanding of how molecules react. It automatically predicts the important reactions and their rates. Use of the RMG reduced initial MPE model development from at least a month of hands-on researcher work to three days of computer processing, saving time and cost. Iterative refinement enables automatic generation of a model that can accurately predict MPE pyrolysis and decomposition during combustion. Researchers are now automating quantum chemical calculations to improve accuracy and speed up the iterative refinement loop. The RMG will significantly reduce the time and expense required for numerical simulations, making it possible to swiftly and effectively generate insight and optimize performance for a broad range of fuels.



Iterative refinement loop for generation of chemical mechanisms using the RMG software. Figure by Max Liu, MIT

Fuel Reactivity Experiments Inform the Development of ACI Engines

Researchers developed a first-of-its-kind approach to measuring the phi-sensitivity (Φ_S) of fuels based on rapid compression machine experiments, furthering the development of a fuel ranking metric and ACI combustion models. Phi-sensitivity, which quantifies the change in a fuel's reactivity as the fuel/air ratio varies owing to stratification within an engine, is important for controlling the operation of ACI engines. No standardized way to measure Φ_S had been reported previously. Phi-sensitivity was measured for the gasoline (10% ethanol blend) RD5-87 at different fuel/air ratios and temperatures under fixed- and varying-pressure protocols. RD5-87 was more reactive as its concentration versus air increased, but the magnitude of sensitivity was substantially lower than that predicted by a Co-Optima kinetic model using the same inputs, implying that model improvements are needed. Further experiments and refinement of phi-sensitivity measurements are underway to better understand how accurately the metric reflects ACI combustion performance.



Measured (circles and squares) and modeled (dashed line) normalized phi-sensitivity vs. temperature for RD5-87. τ = time to fuel autoignition at a particular condition; Φ = actual fuel/air ratio divided by stoichiometric fuel/air ratio. Figure by Scott Goldsborough, ANL

NEXT STEPS

With the completion of boosted spark-ignition (SI) co-optimization research, Co-Optima light-duty activities are transitioning to concentrate on multimode combustion approaches which make use of boosted SI and advanced compression ignition (ACI) combustion modes. Medium-duty (MD) and heavy-duty (HD) work will continue, as researchers wind up their examination of mixing-controlled compression ignition (MCCI) approaches and shift to focus more squarely on ACI combustion.

In Fiscal Year 2019, researchers will:

- Accelerate multimode research and development (R&D) activities, including exploration of lean SI, lean ACI, and dilute stoichiometric ACI approaches
- Complete work on MCCI research, including presenting a final list of MCCI blendstocks with the greatest potential to optimize fuel properties for efficiency, low temperature performance, and emissions reductions
- Expand MD and HD research, including implementation of a joint experimental/modeling approach to systematically and efficiently identify fuel properties impacting ACI combustion
- Factor in the potential impact of electrification when formulating R&D priorities.

Even while pushing into new areas of research, the Co-Optima team will continue to focus on the underlying science needed to supply industry with the knowledge base critical to innovation.

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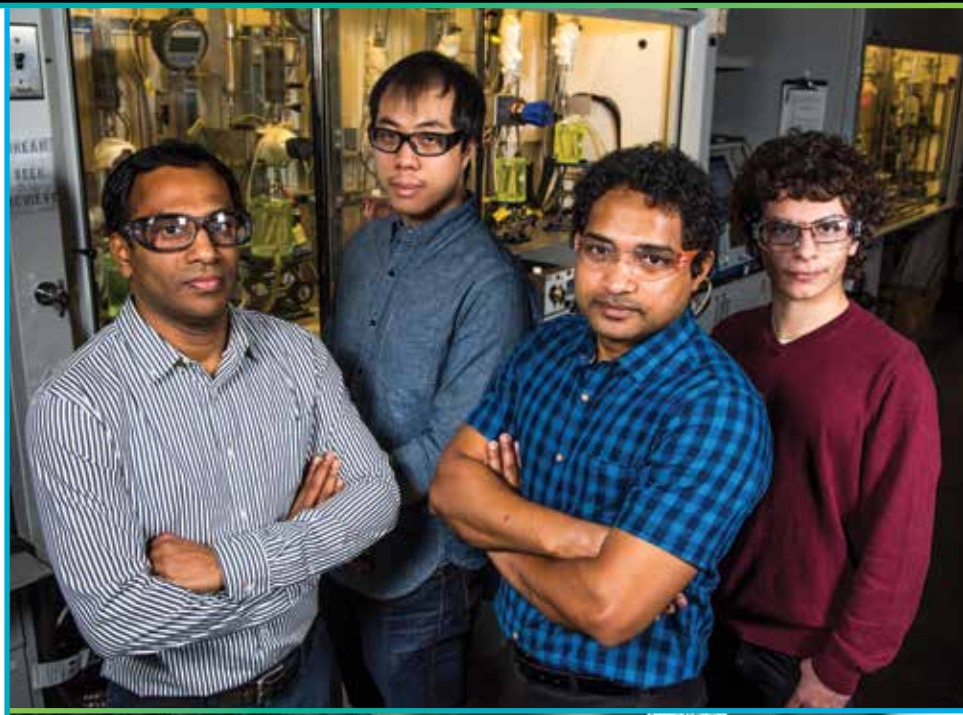

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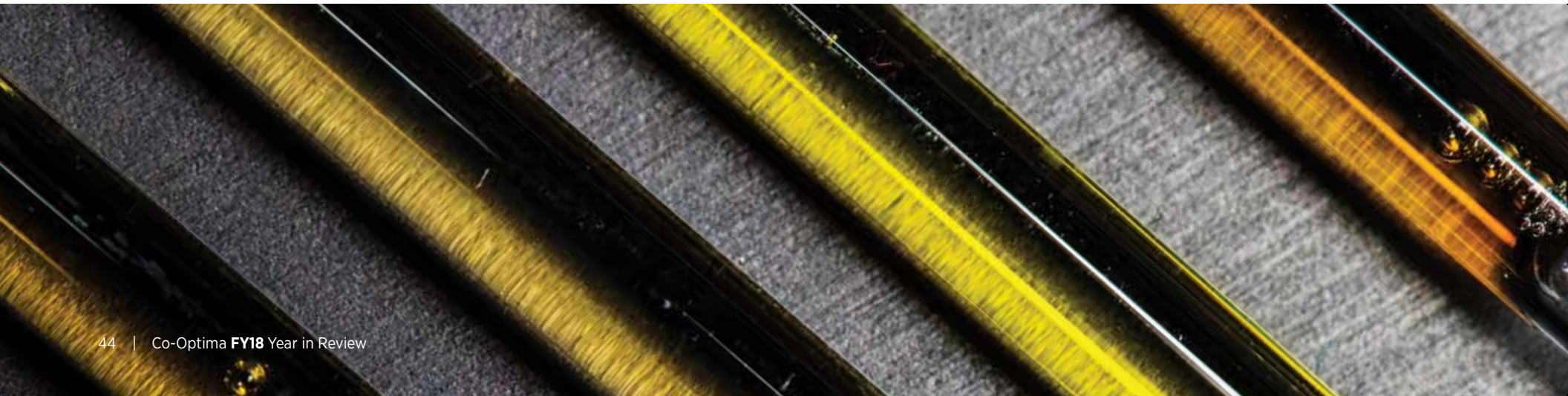

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ACRONYM LIST & GLOSSARY

ACRONYMS & ABBREVIATIONS

3M3P 3-methyl-3-pentanol

ACI ..... advanced compression ignition

AFIDA ..... Advanced Fuel Ignition Delay Analyzer

AKI ..... anti-knock index

ANL ..... Argonne National Laboratory

ARHC ..... aromatic-rich hydrocarbons

ATDC ..... after top dead center

B.P. ..... boiling point

BDC ..... bottom dead center

BDO ..... butanediol

BETO ..... Bioenergy Technologies Office (DOE/EERE)

BOB ..... blendstock for oxygenate blending

C ..... carbon (e.g., C6 = six-carbon)

CA ..... crank angle

CAD ..... crank angle degree

CDC ..... conventional diesel combustion

CFD ..... computational fluid dynamics

CFL ..... Courant-Friedrichs-Lewy

CFR ..... Cooperative Fuels Research

CN ..... cetane number

CO_2e ..... carbon dioxide equivalent

CO ..... carbon monoxide

Co-Optima .... Co-Optimization of Fuels & Engines

CR ..... compression ratio

DCN ..... derived cetane number

DFI ..... ducted fuel injection

DI ..... direct injection

DIB ..... diisobutylene

DOE ..... U.S. Department of Energy

E10 ..... gasoline containing 10% ethanol

E30 ..... gasoline containing 30% ethanol

EC ..... elemental carbon

EERE ..... Office of Energy Efficiency and Renewable Energy (DOE)

EGR ..... exhaust gas recirculation

EPA ..... U.S. Environmental Protection Agency

F.P. ..... freezing point

FAME ..... fatty acid methyl ester

FSN ..... filter smoke number

FY ..... fiscal year

GGE ..... gasoline gallon equivalent

GHG ..... greenhouse gas

HC ..... hydrocarbon

HCCI ..... homogenous charge compression ignition

HD ..... heavy duty

HFS ..... high fuel stratification

HOV ..... heat of vaporization

HRR ..... heat release rate

INL ..... Idaho National Laboratory

IS ..... indicated-specific

K ..... engine-dependent factor in octane index

KI ..... knock intensity

KLSA ..... knock-limited spark advance

kPa ..... kilopascals

LANL ..... Los Alamos National Laboratory

LBNL ..... Lawrence Berkeley National Laboratory

LCA ..... life-cycle analysis

LD ..... light duty

LFS..... laminar flame speed

LHV..... lower heating value

LLNL..... Lawrence Livermore National Laboratory

LT..... low-temperature

MCCI..... mixing-controlled compression ignition

MD..... medium duty

MFSP ..... minimum estimated fuel selling price

MIT..... Massachusetts Institute of Technology

MON ..... motor octane number

MPa..... megapascals

MPE..... methyl-propyl ether

MSS..... Micro Soot Sensor

NMR..... nuclear magnetic resonance

NO_x..... nitrogen oxides

NREL..... National Renewable Energy Laboratory

NTC..... negative temperature coefficient

OC..... organic carbon

OEM..... original equipment manufacturer

OI..... octane index

OMEs..... oxymethylene ethers

ORNL ..... Oak Ridge National Laboratory

P..... pressure

PFS ..... partial fuel stratification

PKS ..... polyketide synthase

PM ..... particulate matter

$PM_{2.5}$..... fine particulate matter

PMI..... particulate matter index

PNNL..... Pacific Northwest National Laboratory

PSHR ..... pre-spark heat release

R&D..... research and development

RCM ..... rapid compression machine

RetSynth..... retrosynthesis

RIM..... refractive index matching

RMG..... Reaction Mechanism Generator

RON..... research octane number

rpm ..... revolutions per minute

RVP..... Reid vapor pressure

S..... octane sensitivity

SI..... spark ignition

SNL ..... Sandia National Laboratories

T..... temperature

TDC..... top dead center

TEA..... techno-economic analysis

THR..... total heat release

TPRF..... toluene primary reference fuel

USCAR..... United States Council for Automotive Research

VTO ..... Vehicle Technologies Office (DOE/EERE)

YSI..... yield sooting index

GLOSSARY

advanced compression ignition (ACI) — A suite of combustion approaches that use compression-induced autoignition to initiate combustion timing, which is controlled by chemical reaction rates (kinetics) rather than by fuel-air mixing

autoignition — Spontaneous ignition of a fuel-air mixture without an external ignition source (e.g., a spark plug)

blendstock — Molecules or mixtures that are combined to make a fuel

boosting/turbocharging — Process in which extra air is forced into the combustion chamber to increase engine efficiency and power

catalyst light-off temperature — Temperature at which pollutants are converted to inert products by emissions-control catalysts

cetane number (CN) — Measure of the ignition quality of diesel fuel; the higher this number, the easier it is to start a standard (direct-injection) diesel engine.

compression ignition — Combustion approaches that achieve autoignition through mixture compression

compression ratio (CR) — Ratio between the volume of the combustion chamber at bottom dead center (fully expanded) and top dead center (fully compressed)

core fuels — Suite of five full-boiling-range gasolines used by Co-Optima researchers to compare results across different laboratories and experimental platforms

direct-injection spark-ignition — Combustion approach in which fuel is injected at high pressure directly into the combustion chamber of an SI engine

ducted fuel injection (DFI) — Method for enhancing fuel-air mixing in MCCI engines by directing fuel sprays into small, co-axial ducts aligned with the spray axes

engine efficiency — Measure of how efficiently an engine converts fuel energy to mechanical work

equivalence ratio (ϕ) — Actual fuel/air ratio divided by stoichiometric fuel/air ratio

flame speed — Speed of flame propagation within an engine cylinder

fuel economy — Measure of how far a vehicle can travel on a set amount of fuel, usually in miles per gallon or miles per GGE

heat of vaporization (HOV) — Energy required to transform a liquid into a gas

homogenous charge compression ignition (HCCI) — Combustion approach in which compressing a well-mixed fuel-air mixture causes autoignition

KL-CA50 — Crank angle where 50% of the fuel has burned under knock limited conditions

knock — Undesired spontaneous ignition of unburned fuel/air mixtures inside engine cylinders that can be damaging to engines

linear blending — Behavior in which the fuel properties of a blended fuel can be accurately estimated by summing the properties of the individual blendstocks multiplied by their relative concentration

merit function — Algebraic equation that quantifies the relationship of key fuel properties to improvements in engine efficiency

mixing-controlled compression ignition (MCCI) — Combustion approach in which ignition timing is controlled by the rate at which fuel and air are mixed to produce a combustible mixture

motor octane number (MON) — Measure of anti-knock quality of a gasoline under relatively severe driving conditions

multimode — Combustion approaches that use different methods of ignition, combustion, and/or fuel preparation depending on engine needs

nonlinear blending — Behavior in which multiple fuel components blended together result in a fuel with properties that are either higher or lower than a linear blending calculation would predict

octane sensitivity (S) — Difference in octane numbers (RON - MON)

particulate matter index (PMI) — Calculated number based on the chemical bond types and vapor pressure of each fuel constituent that correlates with soot PM emissions of fuels

phi-sensitivity — Extent to which a fuel's autoignition reactivity changes as a function of the fuel-air ratio normalized by the stoichiometric fuel-air ratio

RD5-87 — Research gasoline formulation containing 10% ethanol

Reid vapor pressure (RVP) — Measure of fuel volatility

research octane number (RON) — Measure of anti-knock quality of a fuel under moderate/typical driving conditions

soot — Elemental carbon produced in engines from incomplete combustion

spark ignition (SI) — Combustion approach in which a fuel-air mixture is ignited by a spark plug

surrogate fuels — Simple mixtures used to simulate the physical properties and/or chemical reactivity of full-boiling-range fuels

ONGOING DIALOGUE WITH STAKEHOLDERS

The Co-Optima research team recognized from the start that engagement with external stakeholders from industry, government agencies, and research institutions was essential to developing technological innovations with the greatest chance of market impact. "Listening day" events, trade association meetings, individual stakeholder visits, annual merit and peer reviews, and input from Co-Optima's external advisory board have facilitated this critical engagement.

In addition to the two sponsoring EERE offices, nine national labs, and 13 university partners, Co-Optima has engaged with representatives from other government agencies, the petroleum and biofuels industries, automakers and original equipment manufacturers, and trade and consumer groups. In Fiscal Year 2018, a DOE funding opportunity announcement was released to involve more universities and industry entities directly in Co-Optima research pursuits, and the initiative's researchers and management look forward to the awardees joining the team.

Last summer, Co-Optima partnered with the Fuels Institute to host workshops in Detroit and Houston. The gatherings gave stakeholders across the transportation industry a chance to review the latest research on the role of octane and other fuel properties in the design of more efficient engines, as well as exchange thoughts on potential implications for future fuel and vehicle markets.

Co-Optima team members regularly present at conferences and are active participants in professional societies. In FY18, these forums included SAE World Congress, Bioeconomy 2018, Transportation Research Board Annual Meeting, International Summit on Breakout Technologies of Engines and Fuels, IEA Combustion Task Leaders Meeting, American Chemical Society National Meeting, and Green Chemistry Summit.

These exchanges have helped pinpoint research and development (R&D) needs, potential issues, and mitigation strategies in the areas of engine efficiency and performance, fuel production and distribution, infrastructure compatibility, and retail sales. The national labs and EERE recognize that continued exchanges with these partners help focus and prioritize Co-Optima R&D on areas with the greatest chance for near-term market impact, and are vital to the ongoing success of the initiative.

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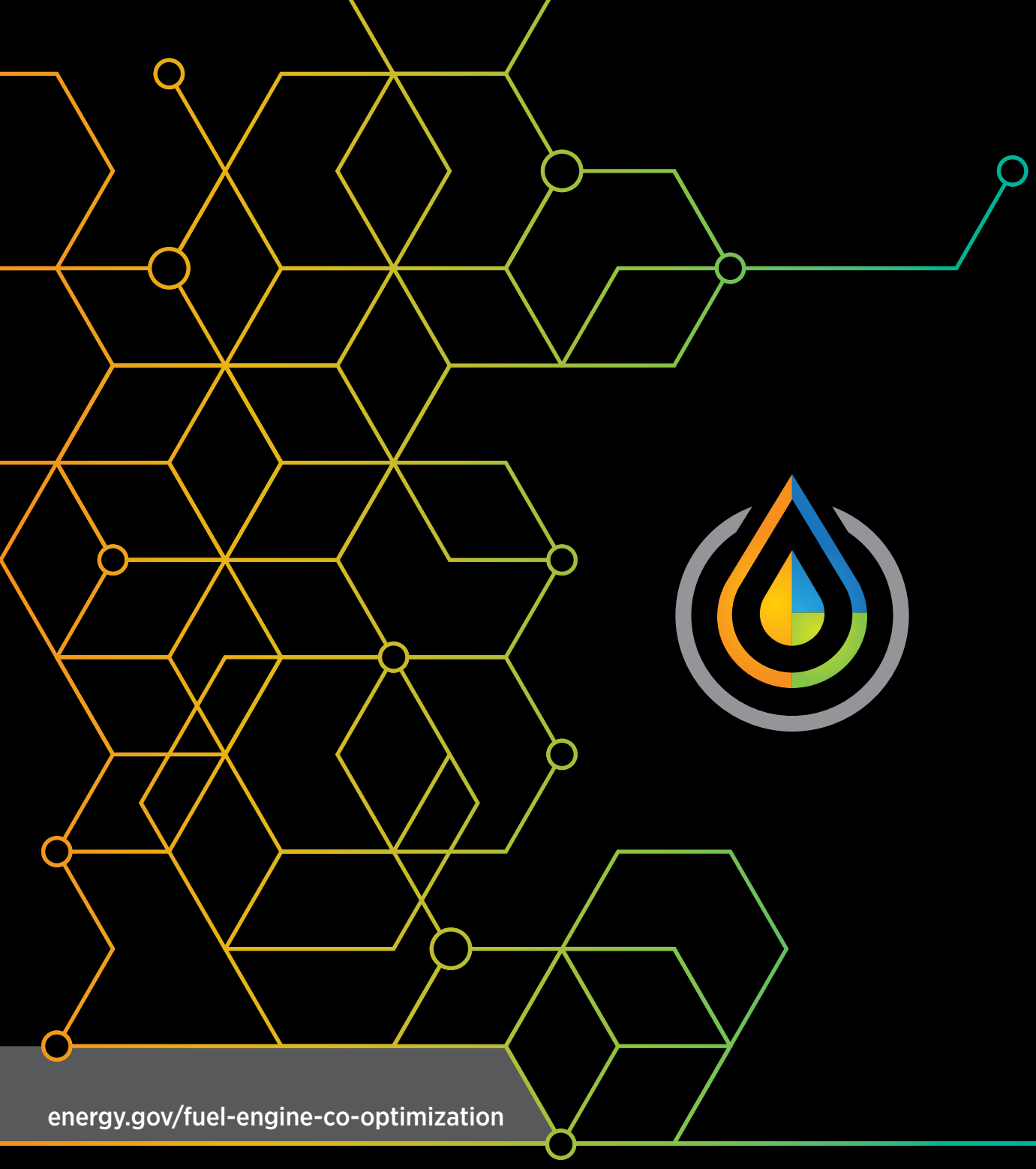

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