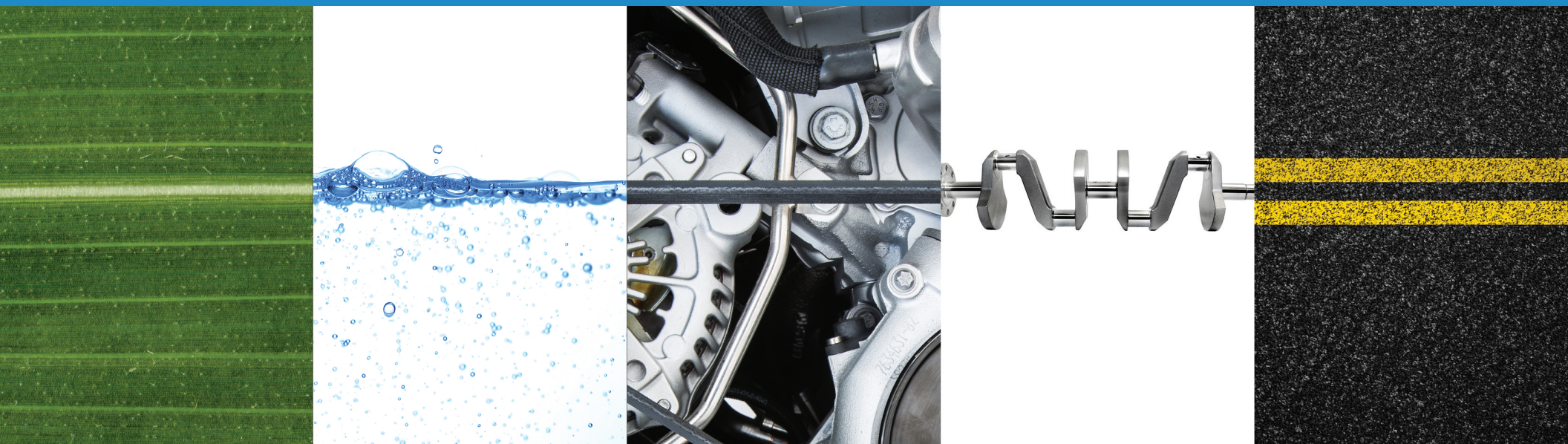
U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

CO-OPTIMIZATION OF FUELS & ENGINES

FY19 YEAR IN REVIEW



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ABOUT THE CO-OPTIMIZATION OF FUELS & ENGINES (CO-OPTIMA) INITIATIVE

The U.S. Department of Energy 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 to maximize light-, medium-, and heavy-duty vehicle fuel economy and performance. The initiative is also mapping lower-cost pathways to reduce emissions while developing knowledge that can be used to leverage diverse domestic fuel resources, boost U.S. economic productivity, and enhance national energy security.

Co-Optima brings together the Bioenergy Technologies (BETO) and Vehicle Technologies Offices (VTO) under the U.S. Department of Energy's Office of Energy Efficiency & Renewable Energy (EERE), nine National Laboratories, and more than 20 university and industry partners. This initiative is targeting solutions with potential to improve today's common fuel and engine types as well as solutions that could lead to revolutionary technologies.

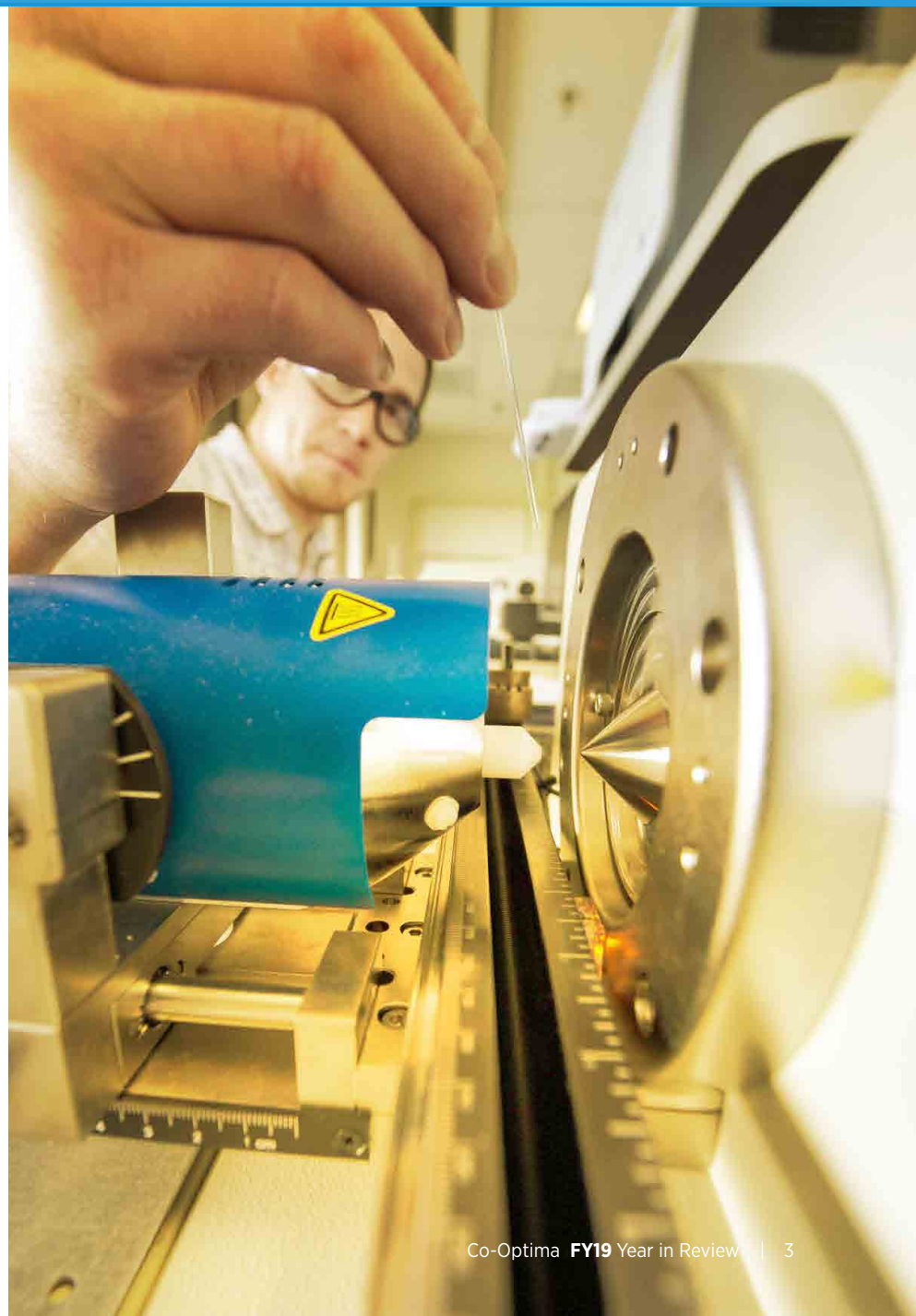
PREFACE

The Co-Optima initiative aligns the expertise and facilities of leading scientists, engineers, and analysts—from National Laboratories and industry and university partners nationwide—to deliver foundational science that is critical to developing fuel and engine technologies working in tandem to achieve efficiency, environmental, and economic goals. The importance of this work is emphasized by recent government and industry projections that show a significant role for liquid fuels and internal combustion engines in transportation continuing for many decades to come. Recent industry interest in low-carbon fuels adds urgency to Co-Optima's efforts. This initiative is providing American industry and policymakers with the knowledge, data, and tools needed to decide which advances could prove most viable and beneficial for drivers, businesses, and the environment.

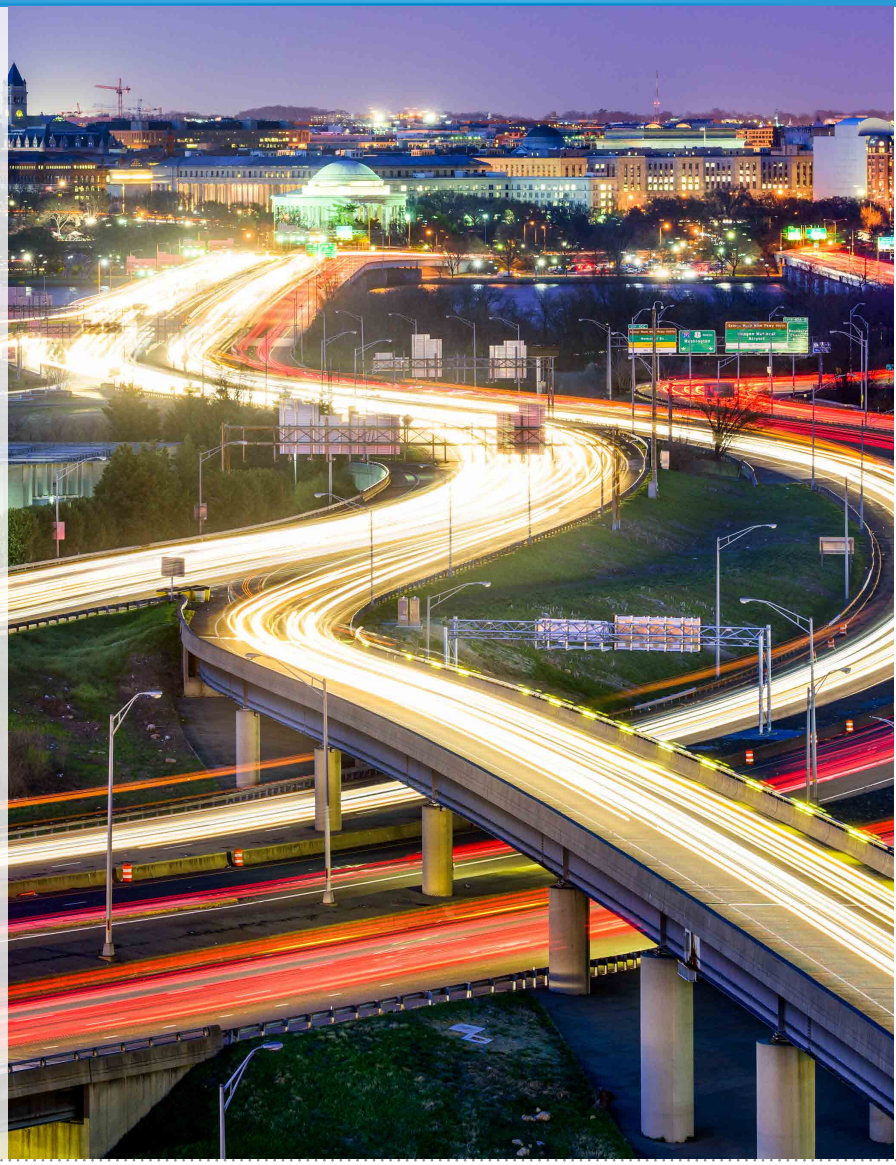
Fiscal year 2019 (FY19) marked the start of Co-Optima's second three-year phase. With boosted spark-ignition (SI) light-duty research completed in FY18, the initiative focused on multimode approaches that combine SI and other forms of combustion—such as advanced compression ignition (ACI)—to increase light-duty vehicle fuel economy. Medium- and heavy-duty transportation research on ACI combustion intensified, while mixing-controlled compression ignition (MCCI) research led to new fuel and combustion insights. One ongoing MCCI research area is ducted fuel injection, a new technology that shows great promise for reducing MCCI engine emissions, especially when combined with oxygenated fuels. We also continue to leverage synergies between the light-duty and medium-duty/heavy-duty ACI research areas to dramatically increase fundamental understanding of fuel molecular structure effects on fuel properties, mixing, soot formation, and autoignition.

This report highlights many of the most significant FY19 accomplishments, including:

- Developing new experimental methods to measure, and models to predict phi sensitivity, an important fuel property for ACI combustion
- Exploring the applicability of an autoignition metric for homogeneous charge compression ignition to other ACI combustion approaches
- Improving computational fluid dynamics simulations to enable exploration of the global sensitivity of ACI operation to fuel and engine parameters



- Combining experiments and simulations of autoignition kinetics to improve kinetic model fidelity and provide new insights into blending effects
- Providing a fresh understanding of fuel chemistry effects on gasoline volatility and evaporation and how gasoline evaporation can impact soot formation
- Generating new data and developing improved methods for predicting molecular structure effects on soot formation
- Completing a sensitivity analysis of ACI combustion for light-duty fuel economy across various engine speeds and load ranges to identify the ranges over which ACI can have maximum impact
- Assessing the potential value to petroleum refiners of biomass-derived blendstocks that enhance the properties of finished fuels
- Identifying promising MCCI blendstocks and performing an MCCI value-proposition analysis to define the opportunities and impacts of new fuels and engines in this sector
- Targeting new fuel molecules with desirable properties for MCCI combustion, leading to multiple new pathways for production of MCCI blendstocks
- Demonstrating orders-of-magnitude lower in-cylinder soot generation in MCCI engines using ducted fuel injection with oxygenated fuels.



These cross-disciplinary accomplishments would not have been possible without aligning the extensive expertise of the multidisciplinary Co-Optima team. This unprecedented level of collaboration has instilled a new spirit of trust and camaraderie across the initiative and fundamentally changed how we work together. We thank the leadership of the Vehicle Technologies Office and Bioenergy Technologies Office—under the U.S. Department of Energy's Office of Energy Efficiency & Renewable Energy—for their vision and support, which have enabled the success of this initiative.

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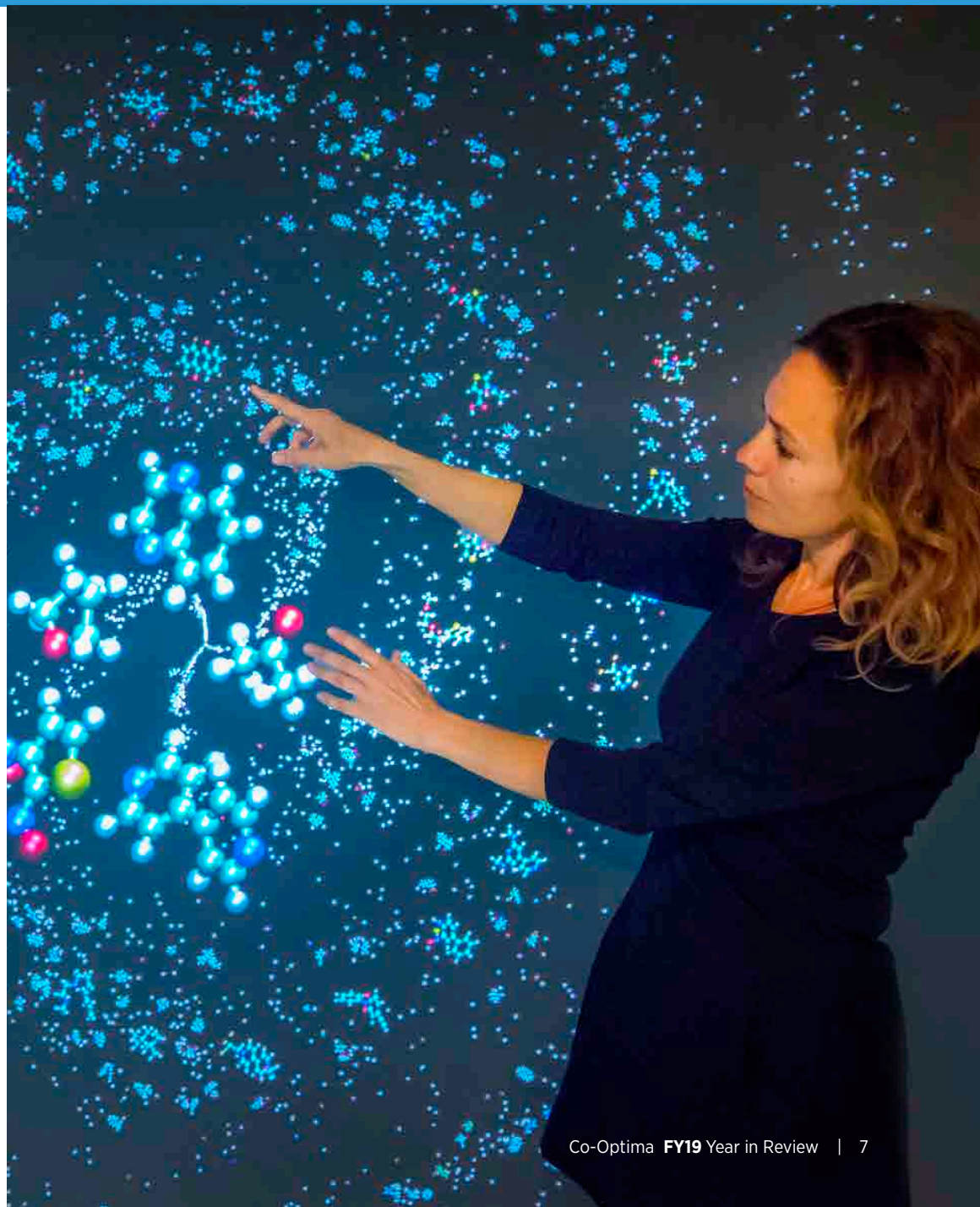
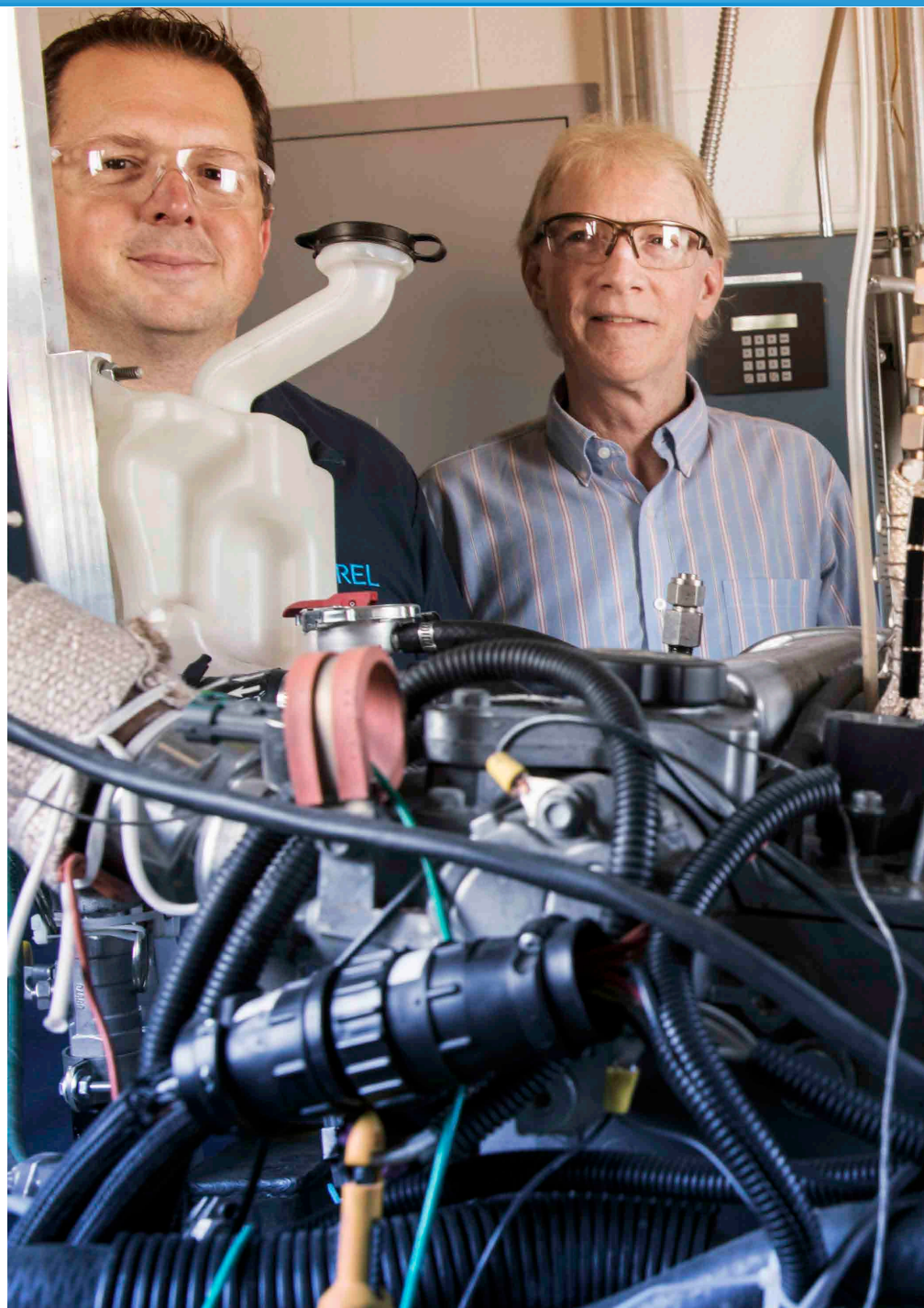


TECHNICAL RESEARCH ACCOMPLISHMENTS AND IMPACT

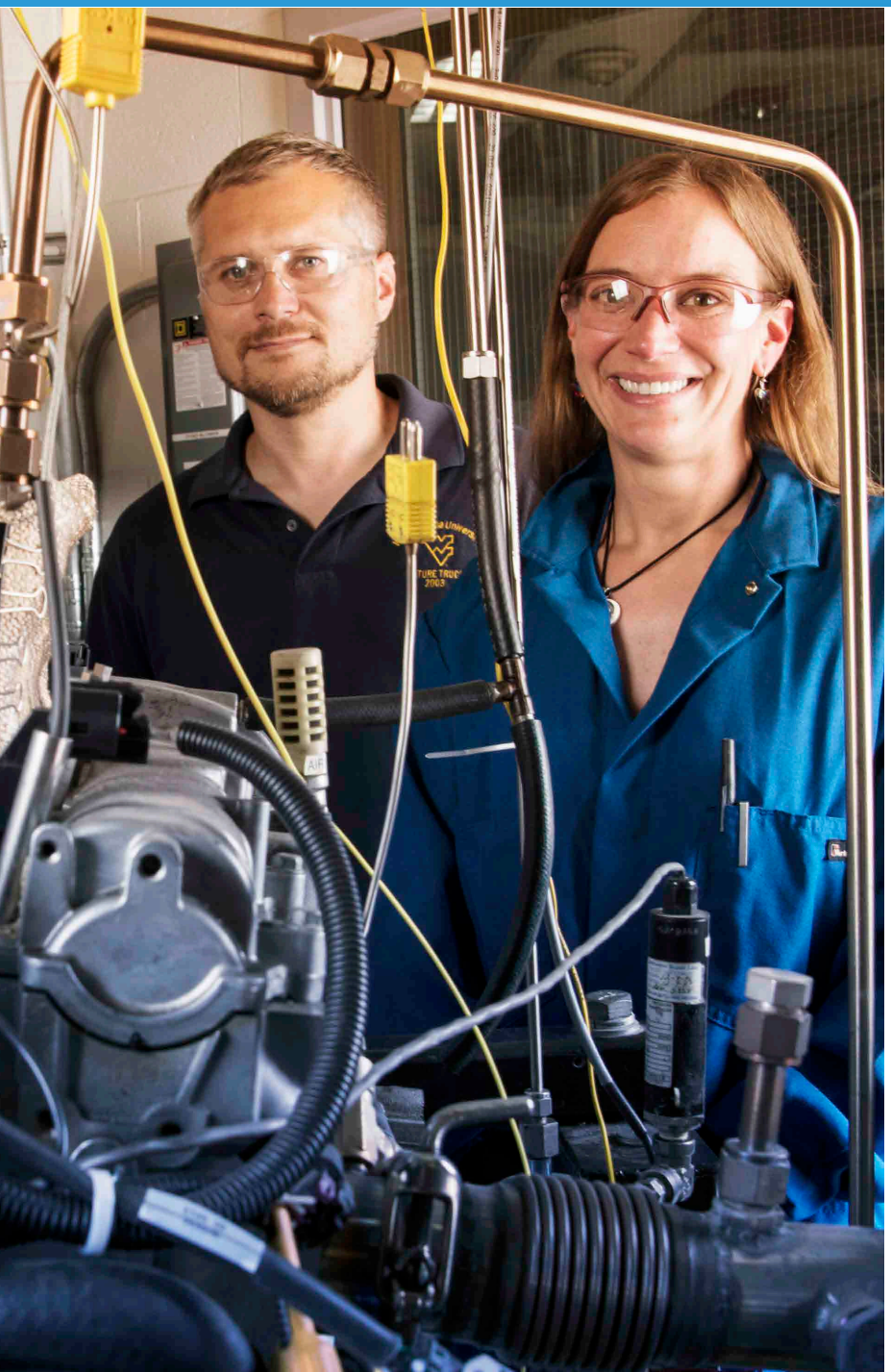
Numerous publications in FY19 followed the FY18 completion of research that showed the impact of fuel properties on efficiency and emissions from boosted SI engines, including a report listing the properties of the top 10 boosted SI blendstocks. In FY19, Co-Optima research transitioned to focus on multimode combustion strategies for light-duty applications as well as MCCI and ACI strategies for medium- and heavy-duty applications.

Co-Optima's consistent focus on research relating fuel chemical structure to fuel properties has accelerated identification and synthesis of potentially beneficial blendstocks through development of a fuel-properties-first approach, in which researchers target molecules with specific fuel properties. This focus has also led to a deeper understanding of soot formation and autoignition chemistry while revealing the boundaries beyond which conventional fuel properties developed for petroleum refinery fuels no longer apply. In particular, Co-Optima has shown that conventional autoignition metrics, such as research octane number and motor octane number, do not predict performance under some multimode combustion conditions. At the same time, Co-Optima analysis has shown the benefit of blendstocks with desirable properties in terms of reduced finished-fuel costs, improved engine efficiency, and lower net-carbon emissions.

Highlights on the following pages represent just a selection of FY19 Co-Optima accomplishments.



LIGHT-DUTY FUEL AND ENGINE RESEARCH



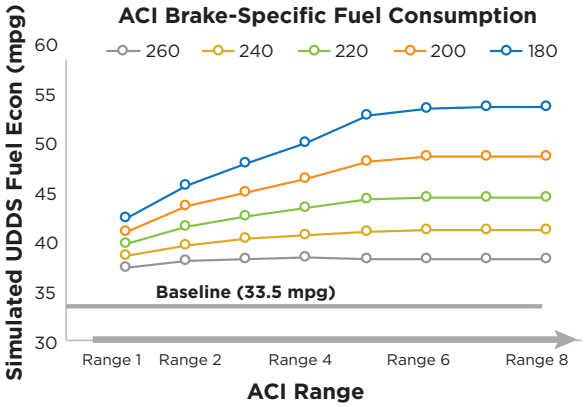
Next-generation engines for light-duty (LD) vehicles may employ more than one combustion mode to achieve higher overall fuel economy. In fiscal year 2019 (FY19), Co-Optima's LD engine research focused on multimode solutions. These solutions employ boosted spark ignition (SI) under high-load conditions, where it is most efficient, and other advanced combustion modes—such as advanced compression ignition (ACI)—under part-load conditions, where boosted SI is less efficient. Lean or exhaust-gas-recirculation dilute ACI combustion has well-documented potential to improve efficiency and emissions under part-load operation, but it poses challenges that limit its use across an engine's speed-load range. Multimode SI/ACI combustion is projected to deliver substantial engine efficiency improvements across the speed-load range while maintaining power density and efficiency gains achieved through downsizing and downspeeding. Research completed in FY19 expanded the understanding of fuel-property impacts on ACI combustion modes relevant to multimode operation. This research focused on fuel-dependent autoignition kinetics, flame initiation and propagation, spray development, mixture formation, combustion development, and soot formation processes.

Previous LD Co-Optima research on boosted SI featured an integrated approach. Critical fuel properties and promising blendstocks were identified. In addition, techno-economic, life-cycle, and refinery integration analyses clarified opportunities for new blendstocks and engine technologies to improve vehicle fuel economy cost effectively. This approach is now being extended to advance next-generation multimode engines.

Select Co-Optima accomplishments related to LD vehicles are found in the following section.

SIMULATIONS CLARIFY ACI RANGE AND EFFICIENCY IMPACTS ON FUEL ECONOMY OF VEHICLES WITH MULTIMODE ENGINES

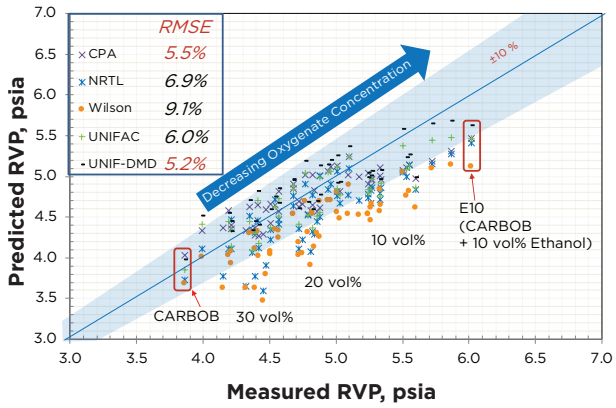
Multimode engines switch between conventional SI and ACI or other lean combustion modes under different operating conditions to achieve higher overall fuel economy. However, the benefits of multimode strategies have not been fully characterized. Co-Optima researchers conducted a systematic simulation study of the effect of ACI engine-map location, load range, and efficiency on the urban fuel economy of an LD vehicle. The researchers used a baseline SI engine map to simulate the baseline fuel economy of a midsized passenger vehicle over a city drive cycle. They then incrementally modified the map with idealized ACI efficiencies in the form of different brake-specific fuel consumption (BSFC) values. For most ACI efficiency cases, fuel economy rose continuously as larger ranges were covered by ACI operation. The increase in fuel economy with increasing ACI load range leveled off in each case because the stoichiometric SI engine was relatively efficient at high loads. In addition, the Urban Dynamometer Driving Schedule (UDDS) used in the simulations includes little driving time at the highest loads. The analysis highlights the magnitude of urban fuel economy improvement that might be realized through multimode engine strategies. It also identifies the low-load engine-map regions where urban ACI operation likely will be most impactful, suggesting prime opportunities for research and development.



Simulated urban fuel economy across ACI ranges and efficiencies—BSFCs of 180 g/kWh (highest efficiency) to 260 g/kWh (lowest efficiency)—in a passenger vehicle with a multimode engine, compared with a baseline vehicle with a direct-injection SI engine. The ranges represent increasing portions of the engine map covered by idealized ACI operation; Range 1 represents the smallest portion covered by ACI (at low loads only), and Range 8 represents the largest portion covered by ACI (across a wide range of loads). Figure by Scott Curran and Robert Wagner, ORNL

PREDICTING RVP OF OXYGENATED FUEL BLENDS FACILITATES ASSESSMENT OF BLENDSTOCK VALUE

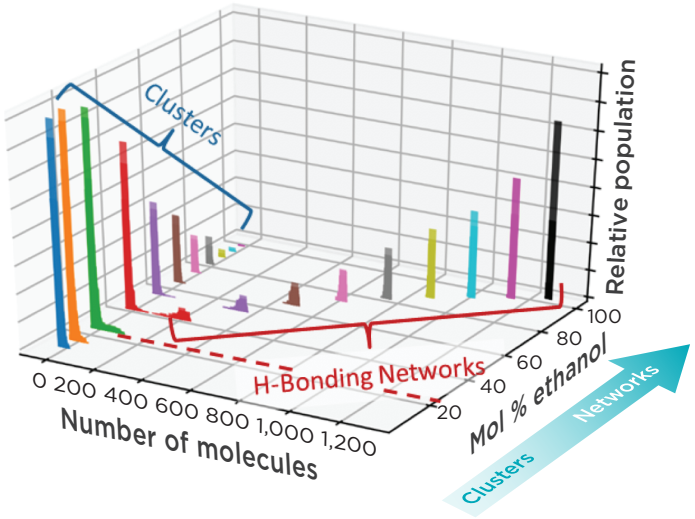
The economic value of a gasoline blendstock is based in part on its impact on Reid vapor pressure (RVP) after blending it with a hydrocarbon blendstock for oxygenate blending (BOB). The ASTM methods used to measure RVP require a small amount of blended fuel for each mixture of interest, which is expensive and time-consuming for research, as well as impractical when inadequate amounts of novel compounds are available. Polar oxygenated compounds tend to have a highly nonlinear blending effect on the RVP when blended with a BOB or a BOB with 10% volume ethanol (E10). Co-Optima researchers developed a computational method using Aspen Plus to predict the RVP of oxygenated fuel blends quickly and inexpensively using several of Aspen's built-in physical property models. The California Reformulated BOB (CARBOB), E10, and oxygenates were modeled using chemicals available in the Aspen Plus physical property database. The method's performance was evaluated by comparing calculated predictions against experimental RVP measurements for various mixtures of oxygenates blended with a CARBOB and an E10 made with the same CARBOB. The results showed that RVP predictions with a root-mean-square error (RMSE) of less than 6% were possible with the method using the Cubic-Plus-Association (CPA) equation of state and the UNIF-DMD (UNIFAC with Dortmund modification) models. These methods facilitate assessment of the commercial value of novel oxygenated blendstocks by quickly predicting the RVP of oxygenate-hydrocarbon mixtures with acceptable accuracy.



Predicted vs. measured RVP at 100°F for 19 oxygenated blendstocks present at 10%–30% by volume in a CARBOB, showing that the CPA and UNIF-DMD predictions are most accurate. The blue line represents perfect prediction (predictions = measured values). Symbols represent predictions of specific activity coefficient or equation-of-state models. NRTL = nonrandom two-liquid activity coefficient model; UNIFAC = UNIQUAC (universal quasichemical) Functional-Group Activity Coefficients; Wilson = Wilson activity coefficient model. Figure by Steven Phillips, PNNL

LINKING ALCOHOL CLUSTERING TO FUEL PROPERTIES SUGGESTS A PATH TOWARD TAILORED BIOFUEL BLENDS

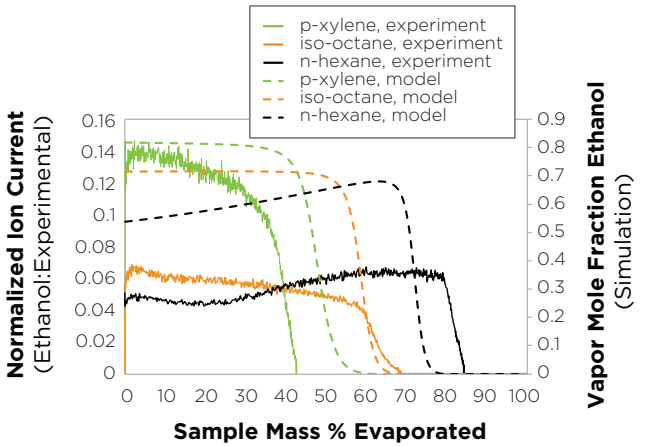
The intermolecular forces among fuel molecules impact macroscopic fuel properties, which in turn affect fuel performance during storage, transport, and use. It is well known that the vapor pressure of gasoline rises significantly when ethanol is added at a low concentration. As the ethanol concentration increases, the vapor pressure rise slows and ultimately decreases below the vapor pressure of the original fuel, in line with the much lower vapor pressure of pure ethanol. To understand the molecular origins of this effect, Co-Optima researchers used a combination of nuclear magnetic resonance diffusion experiments and molecular dynamics simulations. The researchers determined how the structures formed by the alcohol molecules in a hydrocarbon blend change with temperature, concentration, and the species involved. The researchers related blend vapor pressure to the relative amount of the alcohol in hydrogen-bonded clusters and larger networks for ethanol in n-heptane, iso-octane, and gasoline. The results reveal the molecular origins of the vapor pressure changes, opening the door to new strategies to tune the behavior of biofuel blends for improved performance.



Plot of number of ethanol molecules and the fraction of ethanol in clusters or hydrogen-bonding networks as a function of ethanol concentration in n-heptane at 25°C. These molecular dynamics simulation results show the transition from discrete ethanol clusters to hydrogen-bonded ethanol networks beginning at about 20 mol% ethanol (dashed red line). Solution-level organization is dynamic, manifesting as small hydrogen-bonded clusters at low alcohol concentrations and as extensive hydrogen-bonded regions, or networks, at high alcohol concentrations, with a continuum of these species in between. Figure by Amity Andersen, Kee Sung Han, and Tim Bays, PNNL

ALCOHOL EVAPORATION PATTERNS INFORM ENGINE PERFORMANCE AND EMISSIONS PREDICTIONS

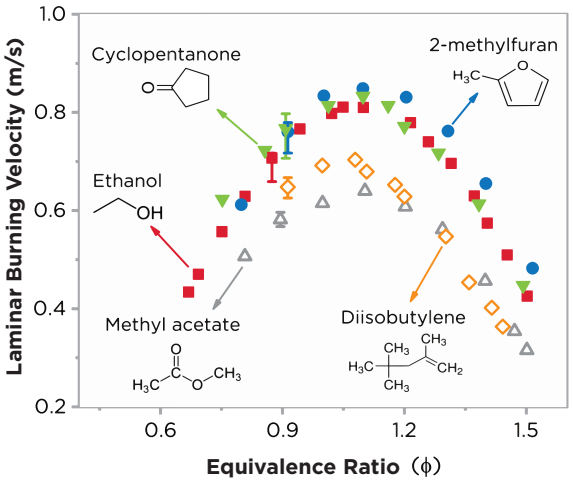
Gasoline-alcohol blend evaporation is dominated by azeotropic interactions that change the evaporation rate, evaporative cooling, and species evolution versus fraction evaporated in comparison to gasoline containing no alcohol. An azeotropic mixture has a constant boiling point and composition throughout its evaporation. Understanding how these effects impact heat and species evolution during fuel evaporation is critical for correctly predicting ignition timing and operability range, and for controlling temperature and phi (fuel-to-air equivalence ratio) stratification and particulate matter emissions. Co-Optima researchers coupled experimental measurements with simulations to investigate which azeotropic interactions between alcohols and gasoline components are most significant. The researchers found that a change in the base composition of the fuel can shift the patterns of alcohol evaporation and related cooling to earlier or later in the evaporation process. To date, ethanol, n-propanol, and isopropanol have been investigated. Results showed an increase in heat of vaporization (HOV) at the point when nearly all the blended alcohol has evaporated—a previously unobserved phenomenon. The HOV increase can delay the evaporation of high-boiling-point aromatic components and consequently increase particulate matter emissions. This research is showing how fuel composition can be used to affect fuel evaporation and emissions.



Vapor composition from UNIFAC equilibrium flash model simulation (right axis, dashed lines, 100 consecutive equilibrium flash stages) and experimental data (left axis, solid lines) for blends containing 50 mol% ethanol, 25 mol% n-octane, and 25 mol% of the target species, showing variable ethanol evolution (as ion current from mass spectrometer) as the sample evaporates. Figure by Gina Fioroni, NREL

LAMINAR BURNING VELOCITY MEASUREMENTS SUPPORT FUEL-SCREENING CRITERIA

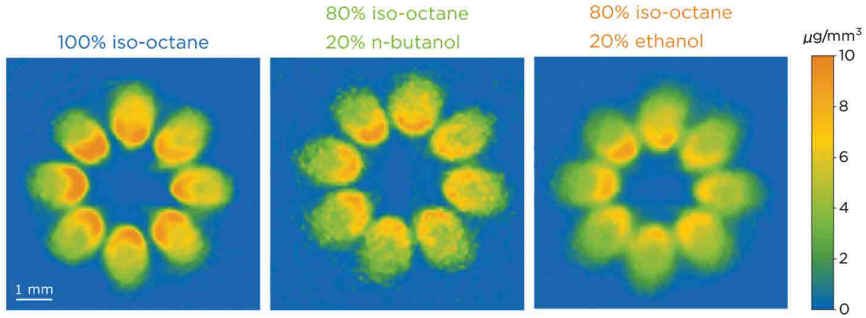
Laminar burning velocity (LBV)—the velocity at which a planar flame progresses through a quiescent fuel-air mixture—affects the rate of combustion in engines and therefore also affects efficiency. The LBV depends on fuel mixture composition, temperature, and pressure, making it a fundamental mixture property and an important target for validation of kinetic mechanisms. LBV is also critical for stable ignition of fuels under lean or highly dilute (high levels of exhaust-gas recirculation) conditions, so it is relevant for both boosted SI and multimode combustion strategies. Co-Optima researchers measured LBV within a constant-volume combustion chamber at initial conditions of 428 K and 1 atm across a range of fuel-to-air equivalence ratio (ϕ) values for five biofuels: ethanol, 2-methylfuran, cyclopentanone, methyl acetate, and diisobutylene. The most important finding is that the LBV values of ethanol, 2-methylfuran, and cyclopentanone were similarly high, while LBV was lowest for methyl acetate, especially under leaner conditions (ϕ < 1). Methyl acetate already had been excluded from further consideration as a Co-Optima blendstock based on its merit function score, a decision further substantiated by its lower LBV. Overall, the current measurements provide critical validation data for ultimately predicting LBV from molecular structure information, while also supporting Co-Optima's criteria for identifying high-performance fuel candidates.



LBV measurements of five biofuel compounds at initial conditions of 428 K and 1 atm. Figure by Subith Vasu, University of Central Florida

X-RAY DIAGNOSTICS QUANTIFY BIOFUEL IMPACTS ON FUEL SPRAY ATOMIZATION

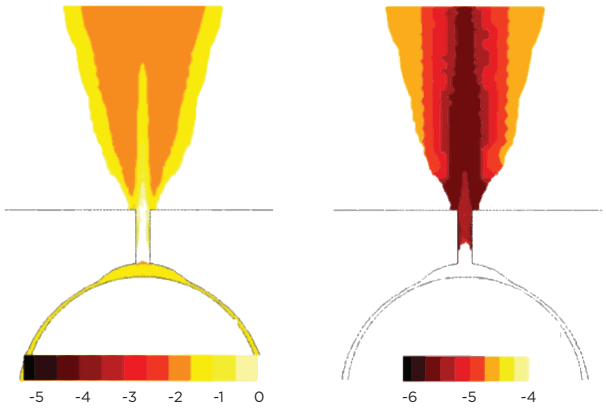
Variations in fuel-injection behavior due to differences in fuel composition create opportunities and challenges for co-optimizing fuels and engines. Co-Optima researchers used unique X-ray diagnostics to quantify changes in the fuel injection process that result when biofuel blends are used in a production gasoline fuel injection system. The measurements were carried out under conditions mimicking those in a real engine at part-load conditions, with hot fuel spraying into a relatively low-pressure environment that causes the fuel to vaporize rapidly, or "flash boil." These extreme conditions are challenging for engine designers because the spray plumes can have a dramatically different structure than at other operating conditions. The measurements revealed that—compared with behavior under high-load conditions—fuel was much more widely dispersed, with a lower overall density throughout the fuel spray. The measurements also quantified the differences between sprays of several biofuel blends, which were caused by different vaporization profiles. Plume spreading was strongest for ethanol mixtures, resulting in plume-to-plume interaction and eventual collapse of the eight individual sprays into a single, narrow, faster-penetrating fuel jet. The measurements quantify the onset of this effect and allow computer simulations of the process to be developed and tested against highly detailed data. With careful design of injection systems, future engines may exploit the sensitivity of the spray structure to fuel composition and optimize fuel and air mixing to enable cleaner-burning, highly efficient combustion.



Tomographic reconstructions of X-ray spray radiography, revealing the density distributions in slices through the sprays from a gasoline injector measured 1.0 mm downstream of the injector. The measurements quantify the differences in spray breakup between the three fuel blends. Figure by Christopher Powell, ANL

LINKING FLASH BOILING TO FUEL PROPERTIES FOR IMPROVED MODELING OF GASOLINE DIRECT INJECTION

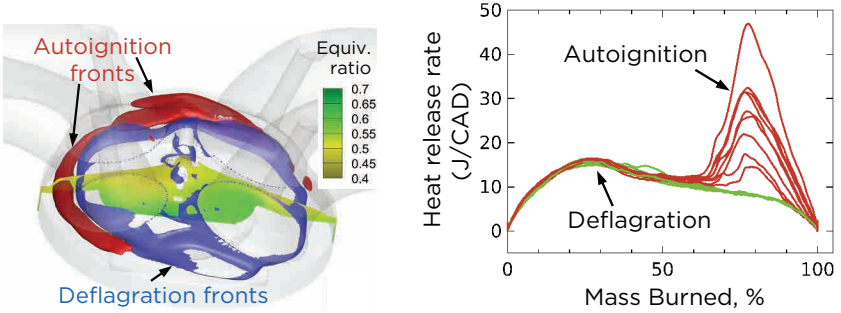
Accurately simulating flash boiling—the rapid vaporization of superheated liquid that occurs in engines at low in-cylinder pressures typical of when gasoline is injected—is important because it affects fuel distribution and ignition conditions. When Co-Optima researchers experimentally measured the boil-off duration for n-pentane, they observed some in-cylinder conditions with significantly shorter boil-off times than those predicted by computational fluid dynamics (CFD) simulations. The researchers determined that the simulations predicted longer boil-off because the correlation used for calculating flash-boiling relaxation time was based on experiments with water. They developed a first-principles derivation directly linking relaxation time to fuel properties by predicting the expansion rate of fuel vapor bubbles inside the superheated liquid phase. A simplified form of the expression was implemented in commercial CFD software as a user-defined function that calculates the flash-boiling relaxation time from the fuel's thermophysical properties. CFD simulations using the new function matched the experimental n-pentane boil-off results more closely. The property-based equations enable prediction of flash boiling for other fuel species and improve the modeling of gasoline direct injection.



Simulated n-pentane flash boiling in simplified injector geometry. Shown are a snapshot based on the standard water-derived relaxation-time correlation (left) and one based on the new Co-Optima function (right). In the logarithmic scales of relaxation time, dark red corresponds to shorter relaxation times (shorter boil-off times), and light yellow corresponds to longer times. Two different scales are used because of the large difference in results. The new function demonstrates rapider, more localized flash boiling for n-pentane, providing an overall better alignment with experimental observations. Figure by Marco Arienti, SNL

COMPUTATIONAL MODEL CAPTURES MIXED-MODE COMBUSTION FEATURES OF SACI ENGINES

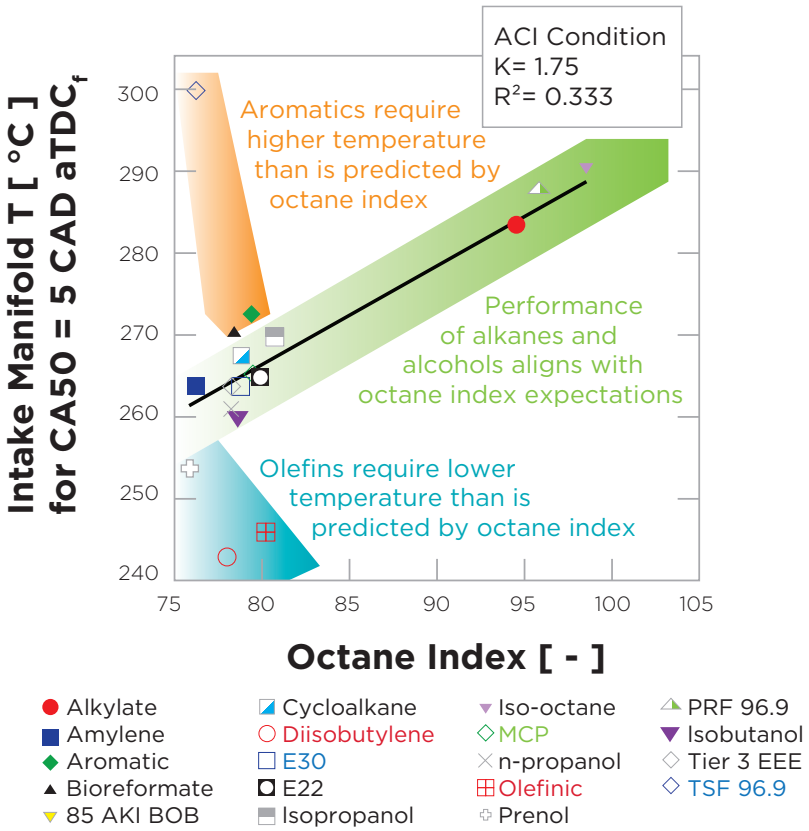
Spark-assisted compression ignition (SACI)—one of several multimode engine approaches—has the potential to improve engine efficiency and performance under a range of operating conditions. Understanding the mechanisms of SACI operation, as well as the relationships between fuel properties and combustion characteristics, is critical to advancing SACI as a multimode technology under the Co-Optima initiative. Researchers developed and validated a computational model that uniquely captures the combination of deflagration and autoignition (mixed-mode combustion) that characterizes SACI engine operation in direct-injection SI engines. Deflagration occurs when injected fuel and air are ignited by a spark, and the resulting flame propagates via diffusion of heat and radicals from the source of the spark. The unreacted gas ahead of this propagating flame, known as end gas, subsequently autoignites when its local pressure and temperature reach a certain threshold. The model of SACI combustion shows that the properties of the fuel, including heat of vaporization and laminar flame speed, influence both types of combustion modes. The computational model also directly quantifies the roles of thermal and mixture stratification and turbulent mixing in the end-gas autoignition process. Ongoing Co-Optima research is characterizing the multimode combustion effects of different fuel types and operating conditions such as partial fuel stratification in premixed charge compression ignition. The resulting computational tools will enhance the understanding of fuel-engine interactions and help identify the optimal fuels for multimode operation.



Left: Simulation of SACI engine operation with E30 (gasoline with 30% ethanol) during mixed deflagration (blue areas) and autoignition (red areas) combustion. The gradient across the center of each simulation represents the equivalence ratio. Right: Heat-release rate (in joules per crank angle degree [CAD]) versus mass of fuel burned for individual engine cycles in the deflagration-only mode (green lines) and the mixed deflagration and autoignition mode (red lines), showing the dominance of autoignition above 50% mass burned in mixed-mode cycles. Figure by Chao Xu, ANL

LINK BETWEEN ACI AUTOIGNITION AND FUEL CHEMICAL FAMILY ADVANCES UNDERSTANDING OF MULTIMODE ENGINES

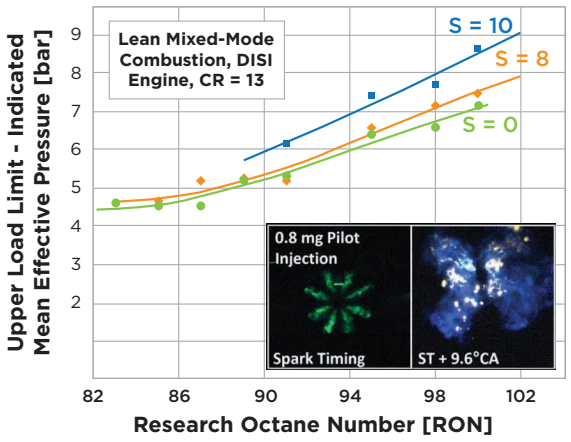
Multimode engines use fuel-lean ACI strategies at part-load conditions to increase efficiency but operate under stoichiometric conditions at high loads to maintain power density relative to modern SI engines. Fuel property metrics that predict fuel performance under both operating modes are needed to specify and supply the fuels required by multimode engines. Co-Optima researchers investigated the applicability of metrics for 19 fuels in a test engine under ACI operation and a range of conventional SI conditions. In agreement with previous literature, under conventional SI conditions the autoignition propensity of the fuels primarily behaved in accordance with the octane index (OI), which depends on the measured research and motor octane numbers but also considers an operating-condition dependency. However, under ACI conditions, the OI metric produced a much poorer correlation, indicating that autoignition propensity is much more dependent on chemical family. Although alcohols and alkanes behaved in accordance with the OI, aromatics required higher temperatures than expected to achieve autoignition, and olefins required lower temperatures. These results support modeling evidence that a chemistry-specific effect not captured by OI or other common ignition metrics is driving performance under these ACI conditions. Co-Optima research is continuing to characterize fuel performance in multimode engines as a way to facilitate development of this promising engine technology.



Required intake manifold temperature vs. OI for 19 different fuels under ACI operating conditions. Vertical axis represents the intake temperature required to burn 50% of the fuel at 5 CAD after top dead center firing (aTDCf). Dark line is linear fit to all points (R^2 = 0.333). Colored fields suggest stronger correlations within fuel families. 85 AKI BOB = blendstock for oxygenate blending with 85 anti-knock index; CA50 = crank angle at which 50% of the fuel has burned; E22 = gasoline with 22% ethanol; EEE = emissions certification fuel; K = factor defining OI at given operating condition; MCP = methylcyclopentane; PRF = primary reference fuel; TSF = toluene standardization fuel. Figure by Jim Szybist, ORNL

MATCHED OCTANE NUMBER AND OCTANE SENSITIVITY REQUIREMENTS OF LEAN SACI AND BOOSTED SI COMBUSTION ENABLE MULTIMODE OPERATION

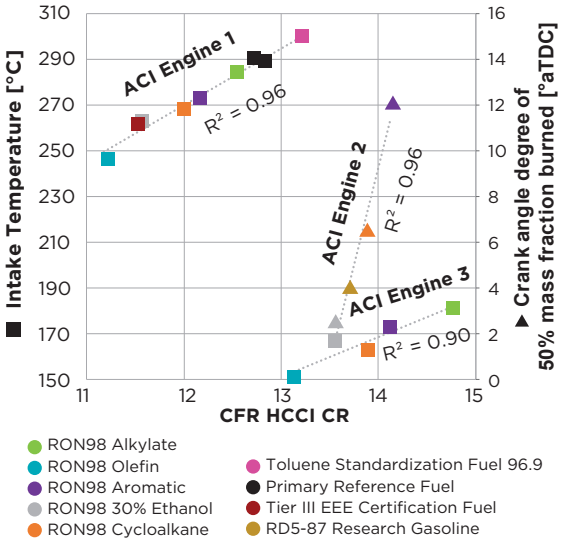
To achieve higher vehicle fuel economy, multimode engines alternate between conventional stoichiometric boosted SI for high loads and ACI or other lean combustion modes at lower loads. Co-Optima researchers combined experiments and modeling to determine the research octane number (RON) and octane sensitivity (S) requirements of SACI mixed-mode combustion in the 1,000–2,000-rpm engine-speed range, which is where engines spend most of their time during typical automotive drive cycles. The results revealed similar RON and S requirements for stoichiometric SI and lean SACI combustion. Both modes allow higher loads to be achieved with fuels having high resistance to autoignition (e.g., high RON and S)—see figure for mixed-mode combustion results at 1,400 rpm. Fuels with high S show less sensitivity to intake boosting and higher compression ratio (CR), thereby further extending the upper load limits of SACI combustion and boosted SI. In these experiments, a small pilot injection of fuel was used to enrich the charge near the centrally located spark plug, which stabilized the flame development for these ultra-lean (λ = normalized air-fuel ratio = 1.8–2.9) SACI operating conditions.



Effect of increasing RON and S on the upper load limit of lean mixed-mode combustion that uses a combination of deflagration (SI) and controlled end-gas autoignition (compression ignition) in a multimode direct-injection SI engine that employs boosted SI for peak loads (indicated mean effective pressure >10 bar) and high engine speeds (>2,000 rpm). Results shown are at 1,400 rpm. The inset illustrates the use of a small pilot injection to stabilize the lean combustion. CA = crank angle; DISI = direct-injection spark ignition; ST = spark timing. Figure by Magnus Sjöberg, SNL

CFR ENGINE HCCI COMPRESSION RATIOS CORRELATE WITH FUEL REACTIVITY IN ACI ENGINES

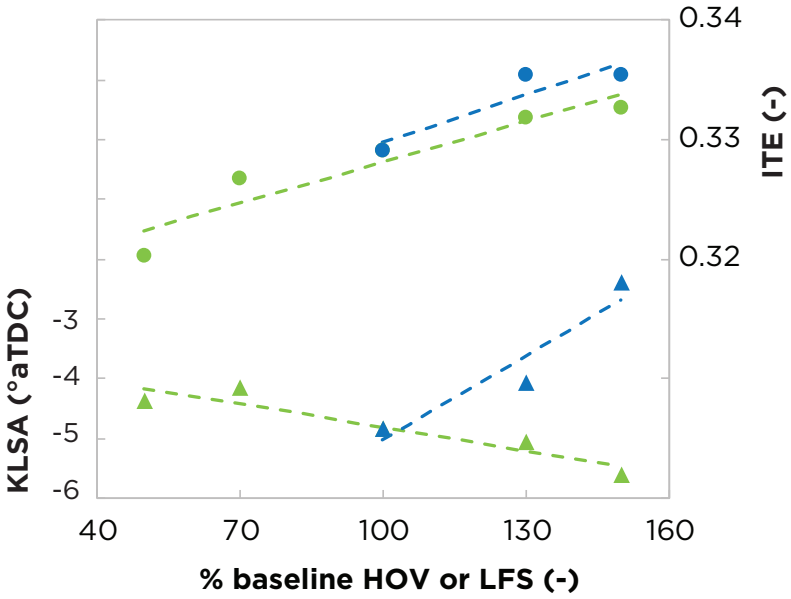
An improved fuel reactivity metric is needed for ACI operation in future high-efficiency engines, because current fuel metrics—RON, motor octane number (MON), and OI, which is derived from RON and MON—do not correlate with reactivity under lean ACI operation. Co-Optima researchers demonstrated the high correlation of Cooperative Fuels Research (CFR) engine CRs with fuel reactivity in three modern ACI engines. The variable-CR CFR engine, the standard engine used for RON and MON tests, can be easily modified to characterize the reactivity of fuels during lean homogeneous charge compression ignition (HCCI) combustion based on the CR required to maintain a constant combustion phasing (CA50 = crank angle at which 50% of the fuel has burned = 3 CAD after top dead center [aTDC]). The researchers found that, under MON-like test conditions (high intake temperature, natural aspiration), CFR engine-based HCCI CRs correlated with HCCI fuel reactivity in modern ACI engines, with R^2 values of 0.9 to 0.96. This high degree of correlation was observed despite variations among the modern engine geometries and operating conditions in terms of engine speed, CR, combustion phasing, and reactivity compensation/rating technique. Using this validated ACI fuel metric based on CFR engine HCCI CRs, Co-Optima researchers can rate and rank the reactivity of fuel components and blends of interest for high-efficiency ACI engines.



Correlation of the CFR HCCI CRs to maintain constant combustion phasing of several fuels (x-axis) to the relevant reactivity metrics in modern ACI engines (y-axes), including intake temperature (squares) and combustion phasing CA50 (triangles). The CR fuel ratings of the CFR engine during HCCI combustion at MON-like conditions correlated very highly ($R^2 > 0.9$) to the fuels' reactivity in modern engines. ACI Engine 1: 2,000 rpm, 1.05–1.15-bar manifold pressure, lambda 3.3, CA50 = 5°aTDC, CR = 13.7:1. ACI Engine 2: 1,200 rpm, 1.0-bar manifold pressure, lambda 2.5, 154°C intake air temperature, CR 14:1. ACI Engine 3: 1,500 rpm, 1.05-bar manifold pressure, lambda 3.3, CA50 = 12°aTDC, CR 15.3:1. °aTDC = CAD aTDC. Figure by Alexander Hoth and Christopher P. Kolodziej, ANL

MODEL ISOLATES EFFECTS OF INDIVIDUAL FUEL PROPERTIES ON BOOSTED SI KNOCK AND EFFICIENCY

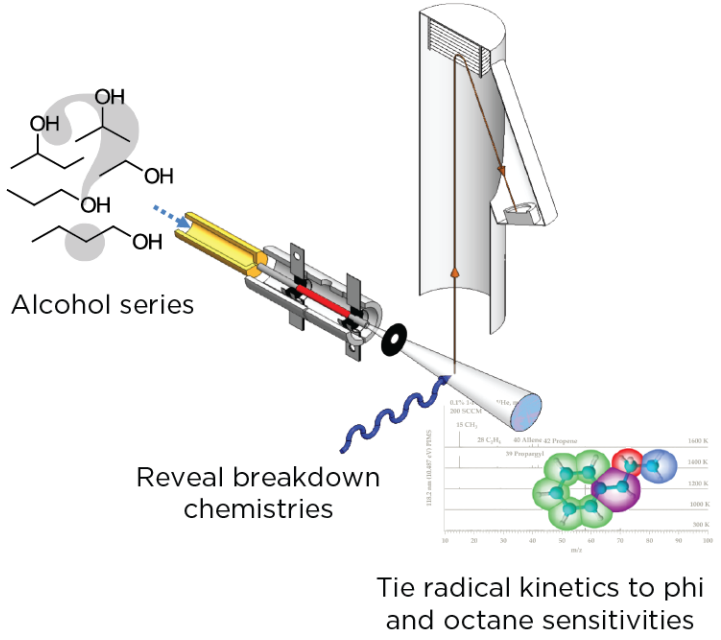
Experimental studies of fuel property effects on engine combustion sometimes produce inconclusive results because of the confounding effects of fuel properties that correlate with one another in complex fuel blends (e.g., gasoline and ethanol), making it difficult to isolate an effect related to an individual fuel property. Co-Optima researchers developed an efficient CFD model to accurately quantify the impacts of fuel properties such as HOV and laminar flame speed (LFS) on engine knock propensity and thermal efficiency. In this model, a transported Livengood-Wu integral approach is used for knock prediction, providing simulation times that are 3 to 10 times faster (less than 8 hours with the new approach on 72 cores per engine cycle) than a pressure-analysis-based approach. This computational method can be used to pinpoint the effects of individual fuel properties, providing specific insights into fuel-engine interactions, supplying a more accurate and comprehensive understanding of how fuel properties affect engine combustion, and helping identify fuels capable of maximizing engine efficiency. For example, the effect of HOV cooling on knock mitigation—which is often considered to contribute to high knock resistance in alcohol fuel—proved to be only moderate within the ±50% HOV perturbation range, and reduced heat transfer because of lower charge temperature was identified as the characteristic most responsible for the efficiency gains seen with higher HOV. Similarly, higher LFS was shown to increase knock tendency and require delayed knock-limited spark advance (KLSA), but indicated thermal efficiency (ITE) was found to increase with higher LFS owing to the reduced combustion duration. The CFD-generated data have been used to validate and update the Co-Optima boosted SI merit function.



Simulated impacts of fuel HOV (green) and LFS (blue) on KLSA (triangles) and ITE (circles) in a boosted SI engine at 2,000 rpm and 120 ft-lb. Symbols represent CFD predictions; dashed lines are linear curve fittings based on those predictions. HOV is varied by ±30% and ±50%, and LFS is varied by 30% and 50% independently. Figure by Zongyu Yue, ANL

COMBINING MICROREACTOR EXPERIMENTS WITH COMPUTATIONAL CHEMISTRY FOR RATIONAL ADVANCED FUEL DESIGN

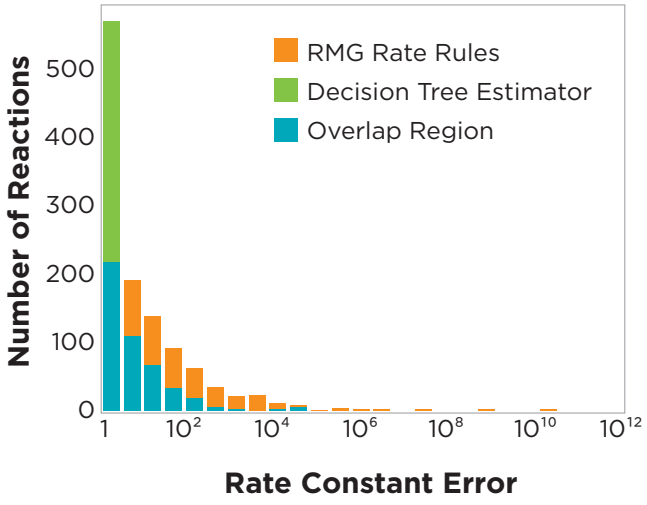
The high-efficiency multimode engine strategies envisioned under Co-Optima will require fuels with octane sensitivity and phi sensitivity to allow control of autoignition under the widely varying combustion conditions of a multimode engine. Drawing on previous Co-Optima work, researchers evaluated the effect of absence or presence of structural features that have been computationally correlated to phi sensitivity (e.g., three CH_2 groups) or octane sensitivity (e.g., primary alcohol). An alcohol series of ethanol to pentanol (linear and branched) was selected for its structural diversity to explore the impact of structure on phi sensitivity and octane sensitivity. The researchers introduced this alcohol series into a microreactor to identify short-lived radical and metastable intermediates by mass spectrometry. Using computational chemistry, these observations can clarify reaction mechanisms and kinetics that are critical to understanding the radical reactions underlying octane sensitivity and phi sensitivity. This work revealed that ignition promotion depends on the initial hydrogen abstraction site, whether the initial abstraction-oxidation step occurs at least two carbons away from the –OH group, and whether the molecule is large enough to offer a choice of ignition-promoting abstraction sites. Where the abstraction occurs determines how oxygen can react with the fuel radical and the population of subsequent products that either enhance ignition (e.g., OH) or suppress ignition (e.g., HO_2). The timing of the production of these species is being correlated with the octane sensitivity and phi sensitivity of these alcohols.



Microreactor experimental approach. Figure by Nabila Huq and Thomas Foust (NREL); Katherine Lockwood, Jatinder Sampathkumar, and Nicole Labbe (CU Boulder)

MACHINE-LEARNING REACTION-RATE ALGORITHM SPEEDS DEVELOPMENT OF BIOFUEL MODELS

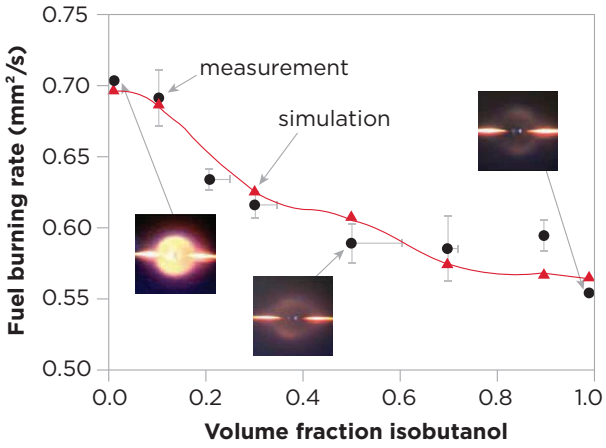
Engine simulations that incorporate high-fidelity kinetics are an important tool for fuel-engine co-optimization. To make useful predictions, biofuel combustion models require fast and accurate estimates of millions of chemical reaction rates. Identifying and correcting errors in these estimates is often the most time-consuming and expensive aspect of model development. Co-Optima researchers addressed this barrier by implementing a more accurate decision-tree-based machine-learning algorithm for chemical reaction rate estimation. In the algorithm, the reaction transition-state structures that have the strongest impact on the rate are automatically identified, and relationships between the heat of reaction and the rate coefficients are fit to groups of reactions with the same important transition-state substructures. The algorithm was trained on rates from the Reaction Mechanism Generator (RMG) database and compared with a much more traditional rate-rule estimator using the same data (see figure). The new algorithm reduced mean absolute errors by about a factor of six. This improved accuracy in rate constants should significantly reduce the amount of effort required to refine models, the need for additional quantum chemical calculations, and ultimately the time and cost required to develop biofuel models.



Accuracy improvements realized using the new decision-tree-based machine-learning algorithm, compared with the traditional RMG rate-rule estimator, for estimating rates of 843 intramolecular endocyclic radical addition reactions. Figure by William Green and Matt Johnson, Massachusetts Institute of Technology

NEW APPROACH FOR VALIDATING COMBUSTION KINETIC MECHANISMS OF BIOFUEL BLENDS IMPROVES ENGINE COMBUSTION MODELING

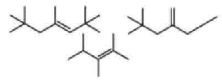
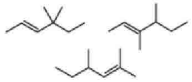
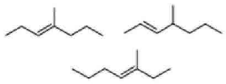
Experimental validation of combustion kinetic mechanisms is critical for developing numerical models of engine combustion. Mechanisms for gasoline-biofuel blends are commonly validated using data from experimental configurations that pre-vaporize the fuel, which eliminates the liquid phase. In real engines, however, liquid fuel injection sets the initial conditions for combustion, and kinetic mechanisms control the heat release rate that influences the fuel burn rate and formation of soot particles. Co-Optima researchers are incorporating the liquid phase into the mechanism-validation process by using a detailed numerical model to simulate data from an experimental configuration based on fuel-droplet behavior. The droplet configuration shares many of the thermal and chemical physics of a fuel-injection spray, such as fuel evaporation, unsteady gas and liquid transport, flame radiation, and formation of soot particles. In a unique facility, test droplets are burned in a sealed chamber under free-fall conditions to eliminate external convection and promote the one-dimensional gas transport needed to generate suitable data. As a first step, the researchers used data from this experimental approach to validate a direct numerical simulation of droplet burning of a model heptane-isobutanol mixture with a known kinetic mechanism. This validation approach will next be applied to isobutanol blended with a gasoline surrogate with an unknown kinetic mechanism, contributing toward combustion modeling that better accounts for liquid injection of biofuel blends.



Data from droplet experiments (black circles) and simulations (red triangles and line) showing accurate predictions of fuel burn rates for heptane-isobutanol mixtures, which decrease with increasing isobutanol concentration. Photographs show soot incandescence from droplet flames decreasing as isobutanol concentration increases, suggesting lower soot particulate formation with increasing isobutanol loading. Figure by Tom Avedisian, Cornell University

CONTROLLING PHI SENSITIVITY VIA ISO-OLEFIN STRUCTURE OPENS ROUTE TO IMPROVED MULTIMODE FUELS

Phi sensitivity quantifies the change in how readily a fuel autoignites as the fuel/air ratio (phi) varies. This variation of ignition delay with phi allows the use of phi stratification (creation of a phi gradient within an engine) to generate sequential autoignition. This reduces pressure rise rate and peak cylinder pressure, and therefore can expand the speed-load range where the high efficiency and low emissions of ACI can be accessed. Iso-olefins have properties well suited for multimode engines—including high RON and octane sensitivity—but the extent to which iso-olefin phi sensitivity can be tailored has been unknown. Co-Optima researchers developed a process to tailor the phi sensitivity of biomass-derived iso-olefins by controlling the degree of iso-olefin branching. The researchers generated mixtures of iso-olefins with one, two, or many methyl substitutions and measured the RON and MON of each mixture. The researchers then used a rapid-compression machine to investigate phi sensitivity. Initial results indicated that modifying the iso-olefin structure changes phi sensitivity, demonstrating that phi sensitivity can be tailored by changing the molecular structure of components of complex mixtures with fuel properties relevant for high-efficiency engines. This capability could facilitate the development of improved fuels for multimode engines. Further research will focus on identifying the specific structural features that govern the relationship between phi sensitivity and iso-olefin structure.

Iso-Olefins Mixture	Research Octane Number	Octane Sensitivity	Phi (ϕ) - sensitivity*
Highly branched 	98	7.9	1.2
Dimethyl-hexenes 	95.2	3.4	1.6
Methyl-olefins 	88.1	2.1	-

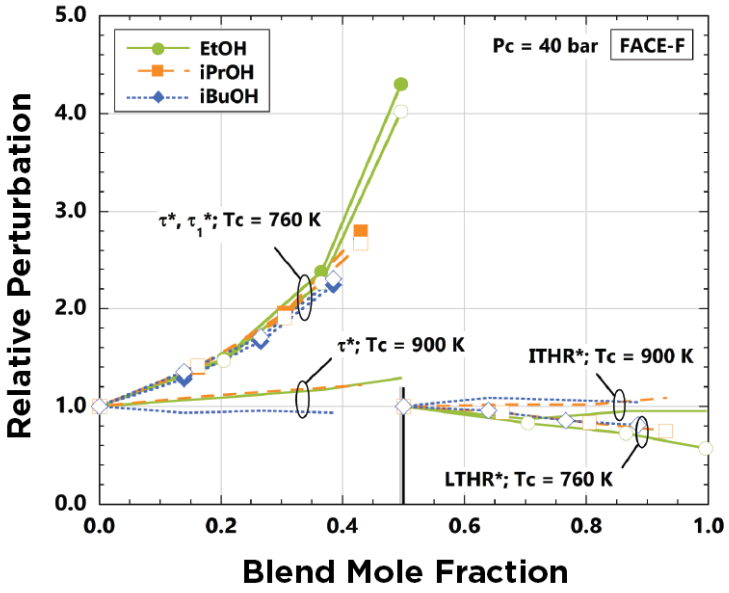
Fuel properties of mixtures of iso-olefins with different degrees of branching (i.e., different numbers of methyl groups). ϕ = fuel-to-air equivalence ratio; τ = ignition delay time, η = ϕ sensitivity metric, a function of temperature (T) and pressure (P). Table by Vanessa Dagle, PNNL

**Phi sensitivity was obtained via rapid-compression machine test and quantified using the following normalized expression:*

$$-\frac{d\log(\tau)}{d\log(\phi)} = -\frac{\phi}{\tau}\frac{d\tau}{d\phi}\Big|_{T,P} = \eta$$

EXPERIMENTS REVEAL BLENDING EFFECTS OF ISOALCOHOLS ON GASOLINE AUTOIGNITION

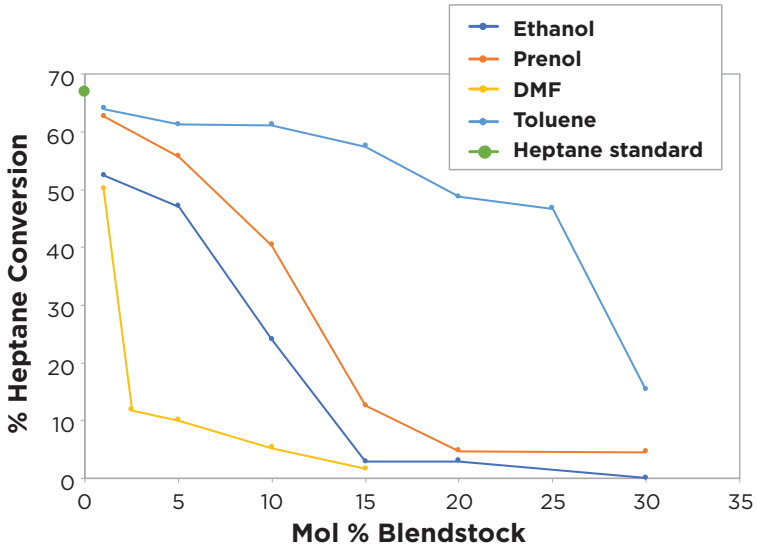
The blending behavior of isoalcohols in gasoline is conventionally established through standardized methods, such as those used to determine RON and MON. However, RON and MON protocols cannot reveal influential properties relevant to multimode and ACI operation, such as low-temperature heat release (LTHR) and intermediate-temperature heat release (ITHR). Co-Optima researchers used a rapid-compression machine to measure the effects of isopropanol (iPrOH) and isobutanol (iBuOH) blending on gasoline autoignition, including shifts in ignition timing and extents of LTHR and ITHR. Changes in autoignition behaviors can affect multimode/ACI engine performance, including load extension and combustion stability, but the chemical effects can be difficult to isolate within the engine environment because of nonuniformities, turbulence, and so forth. FACE-F, one of the Coordinating Research Council's Fuels for Advanced Combustion Engines, was used to represent a research-grade gasoline. The two isoalcohols used in this work are among the top 10 boosted spark-ignition Co-Optima blendstocks, but their blending interactions with petroleum-derived gasolines are not well understood. The assessments covered compressed temperatures (Tc) of 700–1,000 K and compressed pressures (Pc) of 20–40 bar, and comparisons were made to ethanol blending under the same conditions. The results indicated that changes in the autoignition characteristics are more significant at lower temperatures (e.g., Tc = 760 K) than at intermediate temperatures (e.g., Tc = 900 K), suggesting that the isoalcohols will perform like ethanol in multimode/ACI engines. In addition, the blending behaviors among the two isoalcohols and ethanol appeared to be consistent when characterized according to the molar blending fraction, as opposed to the liquid volume fraction. This finding extends prior work comparing the effects of small alcohols (methanol and ethanol), indicating that for larger, three- and four-carbon alcohols, there are generalities in how these potential fuels blend into gasoline.



Shifts in ignition delay times (first stage, τ_1, and main, τ) and early heat release (LTHR and ITHR) as functions of blending mole fractions of ethanol (EtOH), iPrOH, and iBuOH into FACE-F gasoline. Ignition times and heat release are normalized against values for the "neat" fuel (e.g., $\tau^* = \tau_{blend}/\tau_{neat}$). For clarity, the heat release data are shifted to the right on the x-axis by +0.5 mole fraction. Open and filled symbols are first-stage and main ignition results at Tc = 760 K; lines with no symbols are results at Tc = 900 K. Figure by Scott Goldsborough, ANL

FLOW REACTOR STUDIES REVEAL THE CHEMISTRY UNDERLYING SYNERGISTIC BLENDING

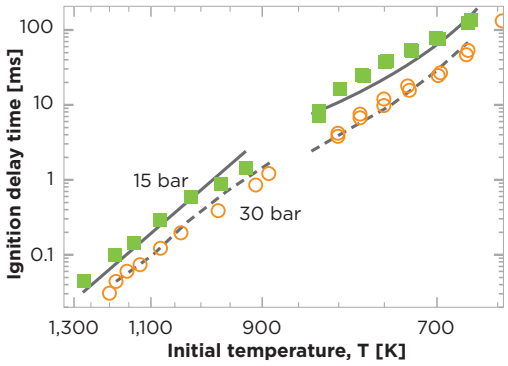
Synergistic (better than linear) blending for RON is exhibited by all of the most promising blendstocks for boosted SI engines and is emerging as an important characteristic of blendstocks for use with multimode engines. High-RON fuels are highly resistant to autoignition, which allows increased CRs and thus higher efficiency. Co-Optima researchers are using flow reactor studies to reveal the chemistry underlying synergistic blending by observing how blendstocks affect the autoignition of heptane, which represents the most reactive component in petroleum refinery-derived gasoline. The blendstocks selected exhibit RON synergy in the following order: ethanol < prenol (3-methyl-2-buten-1-ol) < 2,5-dimethylfuran (DMF). Toluene, a high-RON compound that blends linearly, was included for comparison. DMF began to shut down n-heptane's autoignition at only 1 mol% and dramatically reduced conversion at 2.5 mol%. Observed intermediates and kinetic simulations indicated that hydroxyl and hydroperoxyl radicals generated by n-heptane react with DMF in chain-terminating reactions with low activation energy. Ethanol's effect was similar to DMF's effect at 1 mol%, but adding larger amounts was less effective. Prenol had little effect at 1 mol% and was overall less effective than ethanol. Observed intermediates and simulations showed the formation of chain-terminating species from these blendstocks as well. These species are likely less effective than DMF because they have higher activation energy for these reactions. In contrast, toluene had little effect until 20 mol% had been added, even though toluene's pure component RON value is significantly higher than those for DMF, ethanol, or prenol. Ongoing research is seeking to more quantitatively relate bioblendstocks' radical reactions to RON. A fundamental understanding of synergistic and antagonistic blending for RON will enable design of better bioblendstocks and optimization of refinery blendstocks for oxygenate blending.



The effect of three potential bioblendstocks plus toluene on n-heptane autoignition at a temperature of 600 K, pressure of 1 atm, residence time of 6 sec, and lean conditions. Figure by Robert McCormick and Gina Fioroni, NREL

KINETIC MODEL YIELDS INSIGHT INTO AUTOIGNITION OF PRENOL, A HYPERBOOSTING BLENDSTOCK

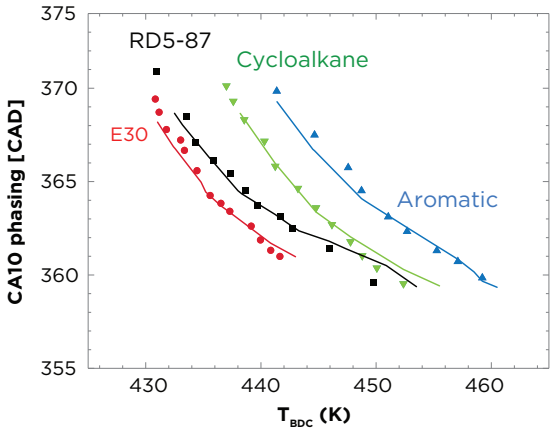
Co-Optima researchers previously identified prenol as a "hyperboosting" blendstock, meaning the RON of prenol-gasoline blends can be higher than the RON of either the neat prenol or the base gasoline by as much as 4.8 octane numbers in some cases. High RON is advantageous for maximizing the performance of highly efficient boosted, high-CR, spark-ignition engines. In their recent work, the researchers developed a kinetic model for prenol by estimating the thermodynamic properties of prenol-related species, analyzing possible reaction pathways, and estimating associated rate constants. They validated the model by comparing simulated results with experimental data from shock tubes, a rapid-compression machine (RCM), a jet-stirred reactor, a flow reactor, and a flame-speed measurement device. Experimental data were obtained from Co-Optima research, the National University of Ireland Galway (NUIG), and existing literature. The figure shows the close agreement between model predictions and experimental measurements in a shock tube and RCM. For neat prenol, short alkyl chains and a highly olefinic nature suppress traditional low-temperature reactivity-enhancing pathways (oxygen addition to fuel radicals and subsequent isomerization), while the hydroxyl group leads to the increased formation of relatively unreactive hydroperoxyl radicals. These structural features inhibit reactivity during combustion at low temperatures for neat prenol, and likely contribute to its high RON, but additional studies of prenol in binary and multicomponent mixtures of gasoline surrogate compounds are required to resolve the fundamental chemistry and physics behind prenol's hyperboosting blending effect on RON.



Simulations (lines) using the Co-Optima kinetic model for prenol and measurements (symbols) of ignition delay times (IDTs) for stoichiometric mixtures of neat prenol in a shock tube (higher-temperature results) and RCM (lower-temperature results). The filled squares and solid lines represent simulations and measurements at 15 bar, and the open circles and dashed lines represent simulations and measurements at 30 bar. The experimental measurements are from NUIG. Interrogation of the kinetic simulations show how structural features of prenol inhibit reactivity at low temperatures, contributing to high RON and RON hyperboosting. Figure by Scott Wagnon, LLNL

KINETIC MODEL ENHANCES PREDICTIONS OF GASOLINE BLENDSTOCK PERFORMANCE IN MULTIMODE AND ACI ENGINES

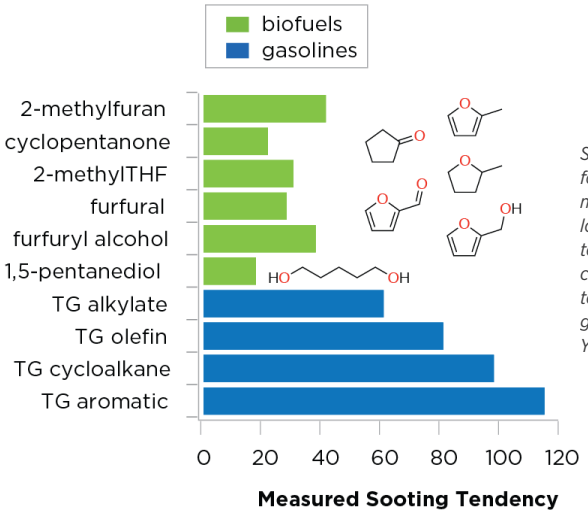
The Co-Optima initiative uses chemical kinetic modeling to identify fuel mixtures with the potential to perform well in multimode and ACI engines—a predictive approach that saves time and resources compared with evaluating many potential fuels experimentally. Researchers improved and validated a detailed chemical kinetic model and developed new surrogate mixtures to represent Co-Optima core gasoline fuels (see figure). The enhanced model uses more fundamental thermodynamic properties for fuel species and kinetic rate constants for reactions to represent the chemistry of surrogate components for gasoline and promising blendstocks. Model results were validated using fundamental combustion data from rapid-compression machines, shock tubes, jet-stirred reactors, and flow reactors provided by Co-Optima research and outside collaborators, as well as from review of existing scientific literature. For example, as shown in the figure, for an HCCI engine, the model predictions for a range of gasoline fuels are typically within approximately 1 CAD of the experimental data from Co-Optima engine researchers. This is a considerable improvement over the previous model, which could only predict within 5 CAD. Co-Optima now has a more predictive chemical kinetic model to simulate the effects of fuels under multimode and ACI engine regimes.



Comparison of simulation results from the improved chemical kinetic model using new seven- to nine-component surrogate blends (lines) and experimental data (symbols) for ignition phasing of gasoline fuels in an HCCI engine. RD5-87 is an 87 anti-knock index gasoline representing an E10 market fuel. Other fuels are Co-Optima core gasoline fuels with different chemical compositions but with the same research octane number of 98 and octane sensitivity of 10. CA10 = ignition phasing of 10% heat release; T_{BDC} = temperature when the piston is in the bottom dead center position. Figure by Dario Lopez-Pintor and John Dec, SNL

BIOFUELS FROM LIGNOCELLULOSE DEMONSTRATE LOW SOOTING TENDENCIES COMPARED WITH GASOLINES

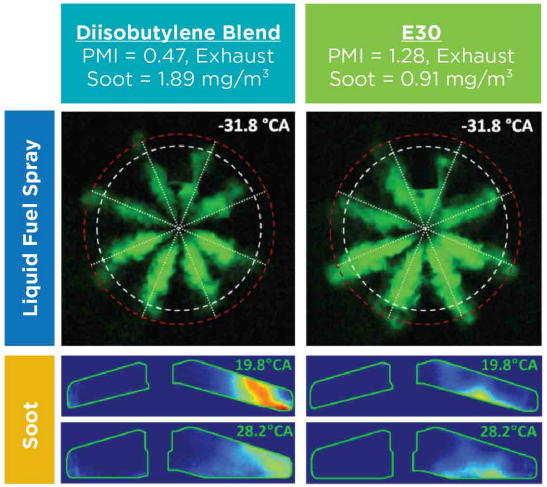
Biofuels could provide a low-cost pathway to meeting particulate emissions standards. However, a wide range of potential fuels can be made from lignocellulosic sugars by various biorefinery upgrading pathways—including furans, cyclic ketones, alcohols, and diols—and testing the emissions performance of all these candidates in real engines is not feasible. Engine studies are time intensive, and the large fuel samples required are inordinately expensive for initial screening purposes. To overcome these issues, Co-Optima researchers developed a novel procedure that quantifies fuel-sooting tendencies at the laboratory scale with high throughput and sample volumes of only 100 microliters. The researchers used this method to compare sugar-derived SI bioblendstocks with gasolines. Because gasoline does not have a fixed composition, the researchers used a suite of test gasolines developed for the Co-Optima initiative, which have a range of compositions that bracket today's market fuels. The measurements demonstrated that many of the biofuel molecules generated less soot compared with all of the gasolines, including the six shown in the figure. Two of these low-sooting biofuels—the furan mixture and cyclopentanone—are among the top 10 SI blendstocks identified by Co-Optima as having the potential to increase engine efficiency by 10%. The emissions benefits of these high-engine-efficiency blendstocks could speed their adoption in the marketplace.



Sooting tendencies measured for several lignocellulosic biofuel molecules that had particularly low values, and for the Co-Optima test gasolines. A larger value corresponds to a sootier fuel. THF = tetrahydrofuran; TG = Co-Optima test gasolines. Figure by Charles McEnally, Yale University

EXPERIMENTS SUGGEST NEED FOR NEW METRICS TO PREDICT SOOTING UNDER LEAN-STRATIFIED SI ENGINE OPERATION

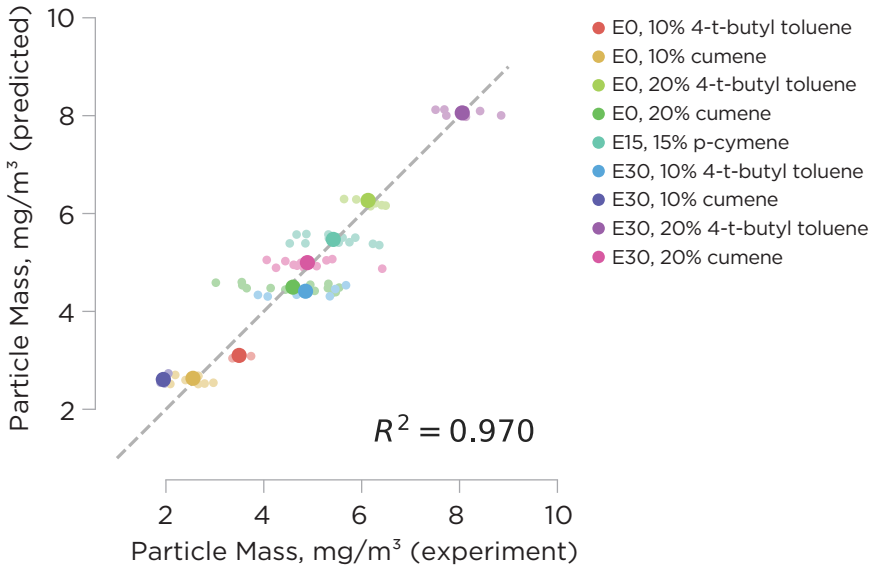
Ensuring clean combustion is imperative when fuels and engines are codeveloped for high efficiency. This requires understanding the sooting propensity of new fuels. Co-Optima researchers assessed the ability of particulate matter index (PMI), a commonly used sooting metric for stoichiometric SI combustion, to predict engine-out soot mass for nine fuels across three well-mixed stoichiometric and two lean-stratified operating strategies. The engine experiments confirmed that PMI works well for conventional steady-state stoichiometric operation but revealed shortcomings under lean-stratified conditions. Specifically, for a slightly boosted stratified-charge operating condition, a volatile surrogate fuel blend with 20% diisobutylene (DIB) showed higher exhaust-soot mass than expected based on its low PMI, while a full-boiling-range E30 gasoline showed lower soot mass. In-cylinder optical soot and spray diagnostics showed that the liquid spray development was very similar for the two biofuel blends (upper images), while in-cylinder soot levels (lower images) scaled with the exhaust-soot mass level. These observations point to an inability of PMI to correctly predict in-cylinder soot formation as fuel composition changes under lean, stratified conditions; that is, these deviations do not appear to stem from differences in soot oxidation or strong fuel effects on the liquid sprays. The results suggest that further work is required to develop a fuel-property metric for sooting propensity that can cover advanced lean combustion.



In-cylinder spray (viewed from below) and soot (viewed from the side) for lean-stratified operation using a DIB blend and E30. Conditions: 2,000 rpm, intake pressure = 130 kPa, intake oxygen mole fraction = 17%, λ (normalized air-fuel ratio) = 3. Figure by Namho Kim, SNL

RESEARCH CLARIFIES ETHANOL'S CONTRADICTORY EFFECTS ON GASOLINE PM EMISSIONS

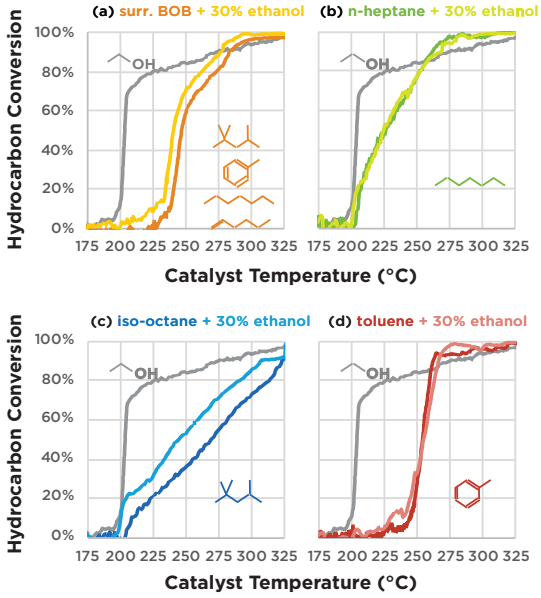
Blending ethanol into gasoline is expected to reduce particulate matter (PM) emissions from SI engines, because ethanol dilutes the aromatics in gasoline that are the primary source of PM. However, literature reports that blending ethanol in gasoline increases PM emissions in some cases, while reducing it in others. Co-Optima researchers used a designed fuel matrix (varying ethanol and aromatic content as well as aromatic vapor pressure) to provide a scientific explanation for these contradictory findings, along with a better PM predictive model. New analytical chemistry techniques and single-droplet fuel evaporation modeling showed that ethanol affects hydrocarbon vapor-liquid equilibria, which inhibits aromatics' evaporation and concentrates aromatics in the shrinking fuel droplets. Coupled with increased evaporative cooling from ethanol, this phenomenon leads to longer droplet lifetimes and aromatic enrichment in the evaporating droplets. These inhibitory effects compete with aromatics' dilution from ethanol blending. Consequently, when fuels containing a low-vapor-pressure aromatic (4-t-butyl toluene) were combusted in a direct-injection SI engine at high speed and load, ethanol blending significantly increased PM emissions, as predicted. However, under the same engine conditions, PM emissions proved insensitive to ethanol blending for fuels containing a higher-vapor-pressure aromatic (cumene), demonstrating that ethanol's dilution and inhibitory effects were balanced. Ethanol's dilution effect fully manifested as significantly reduced PM emissions when the concentration of the higher-vapor-pressure aromatic was lowered from 20% to 10%. This research provides guidance for improving gasoline blendstocks for oxygenate blending that will reduce PM emissions when blended with ethanol.



Validation of the improved ethanol-gasoline PM predictive model, which incorporates an ethanol-aromatic interaction term and aromatic yield sooting index. E0, E15, E30 = gasoline with 0%, 15%, and 30% ethanol, respectively. Figure by Peter St. John, NREL

AROMATICS INHIBIT CATALYTIC CONVERSION OF REACTIVE BLENDSTOCKS AND DIMINISH COLD-START EMISSIONS BENEFITS OF OXYGENATED FUELS

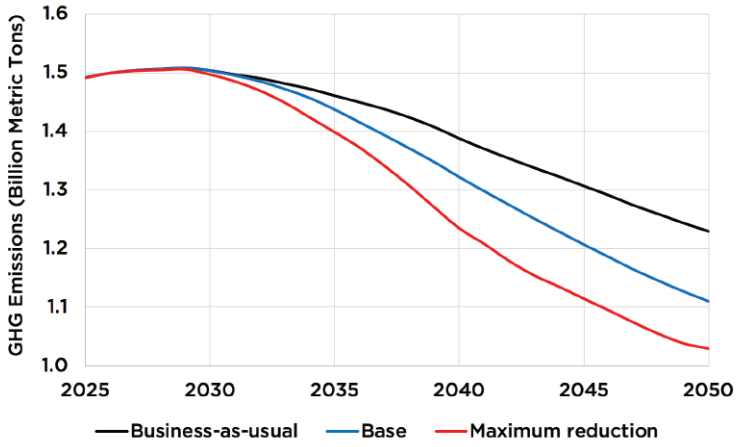
One potential benefit of the Co-Optima initiative is the identification of fuels that reduce cold-start emissions through lower emissions-control catalyst light-off temperatures. Previous research demonstrated that some oxygenated blendstocks, such as ethanol, have low light-off temperatures in their pure form. However, blending the reactive oxygenates into a gasoline surrogate largely eliminated their light-off performance benefits. In a follow-on study, researchers used binary blends of the gasoline surrogate constituents with ethanol to understand these trends. Mixtures of ethanol with alkanes (iso-octane and n-heptane) showed hydrocarbon conversion at temperatures similar to those at which pure ethanol lights off, indicating that the ethanol in the mixtures was reacting over the catalyst. However, the mixtures of ethanol in toluene and in the surrogate BOB, which contained 25% toluene, did not light off until much higher temperatures, indicating that toluene inhibits the catalytic reactivity of more reactive blendstocks. The results suggest that exploiting the lower catalytic light-off temperature of oxygenated blendstocks to reduce cold-start emissions would require reducing the toluene and possibly other aromatic hydrocarbons in fuels.



Hydrocarbon conversion vs. catalyst temperature for pure fuel components (dark colored lines) and 30% ethanol blends (light colored lines) with (a) a surrogate BOB containing 55% iso-octane, 25% toluene, 15% n-heptane, and 5% 1-hexene; (b) n-heptane; (c) iso-octane; and (d) toluene. The conversion of pure ethanol is denoted by the gray line in each chart, and the chemical structures of the fuel components in each experiment are shown within their respective charts. Figure by Josh Pihl, ORNL

BOOSTED SI ENGINES CO-OPTIMIZED WITH BIOBLENDSTOCKS COULD PROVIDE 16% ANNUAL GHG REDUCTION BY 2050

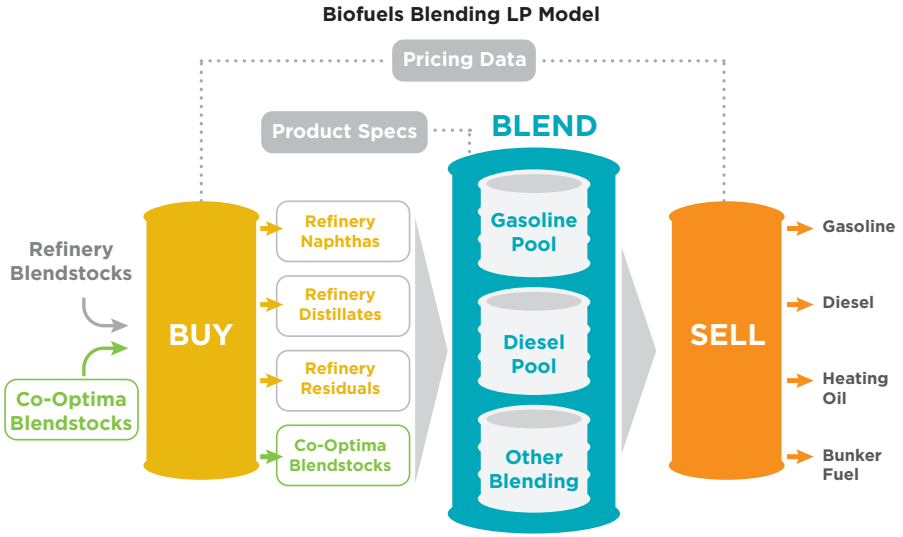
Co-Optima analysis illustrated the critical role bioblendstocks can play in large-scale deployment of co-optimized fuels and engines, decreasing the energy use and negative environmental effects of the LD vehicle fleet. Researchers considered isopropanol blended at 30%, a methylfuran mixture blended at 15%, and ethanol blended at 17%. At these blending levels, each blendstock has the potential to increase the efficiency of a boosted SI engine by 10% over baseline gasoline (i.e., regular gasoline blended with 10% ethanol). The analysis used modeling and analytical tools—including the Automotive Deployment Options Projection Tool (ADOPT); the Biomass Scenario Model (BSM); the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET™) model; and the Bioeconomy Air emissions, Greenhouse gas emissions, and Energy consumption (Bioeconomy AGE) model—to characterize changes in the U.S. LD vehicle fleet through 2050 based on 2025 adoption of the three blended fuels under examination, along with co-optimized engines. Results for the isopropanol blend indicated greenhouse gas (GHG) reductions of as much as 7% cumulatively between 2025 and 2050 and an annual reduction of up to 16% in 2050 compared to the business-as-usual scenario. Annual reductions continue to grow if the analysis is carried beyond 2050.



GHG emissions reductions for the U.S. LD fleet when engines are co-optimized with a 30% isopropanol blended fuel to achieve a 10% engine efficiency gain in 2025. Base emissions assume the LD fleet evolves per market demand. Maximum emission reduction assumes that the fleet transitions completely to co-optimized vehicles over time. Figure by Hao Cai, ANL

CO-OPTIMA SI BIOBLENDSTOCKS PROVIDE ECONOMIC VALUE FOR REFINERS

Various bioblendstocks demonstrate synergistic effects and a significant enhancement in properties when blended with petroleum blendstocks. To understand the opportunities of these bioblendstocks in fuel markets, their value to petroleum refiners must be estimated, which can be complemented by further studies of market dynamics. Using tools and methods aligned with those of the refining industry, Co-Optima researchers evaluated the economic value to refiners of six boosted SI Co-Optima bioblendstocks: i-propanol, n-propanol, i-butanol, diisobutylene, cyclopentanone, and a 40/60 mixture of methylfuran and dimethylfuran. Two approaches based on linear programming (LP) modeling—blending optimization and a full-scale refinery model—were developed to translate the bioblendstocks' superior properties into opportunities to improve the profitability of petroleum-refining processes. Based on the first blending optimization study, the economic value of the bioblendstocks ranged from $2.2 to $4.0 per gasoline gallon equivalent. The value depends strongly on bioblendstock properties (especially research octane number), fuel specifications, and the market prices of petroleum-derived fuels. The researchers have also identified additional representative refinery configurations that can be leveraged to rigorously evaluate opportunities for Co-Optima bioblendstocks in relation to their effects on refinery operations and value.



Schematic of the blending optimization approach employed to estimate the value of Co-Optima blendstocks. Figure by Avantika Singh (NREL), Yuan Jiang (PNNL), and Sue Jones (PNNL)

MEDIUM- AND HEAVY-DUTY FUEL AND ENGINE RESEARCH

Co-Optima research is targeting solutions that will impact the entire on-road fleet, including technologies needed to improve medium- and heavy-duty vehicle performance while reducing emissions. These efforts include two major approaches spanning mixing-controlled compression ignition (MCCI) and advanced compression ignition (ACI) combustion concepts.

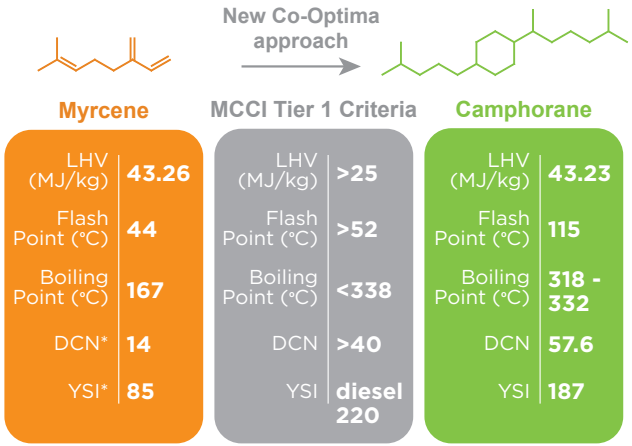
Diesel-fueled engines using MCCI combustion, which are widely employed for commercial transportation, are extremely efficient but require costly emissions-control technologies. Improved MCCI technologies and low-net-carbon blendstocks hold potential to balance high efficiency with reduced engine-out emissions while maintaining critical fuel characteristics, including high energy density, which is important for commercial applications. Major Co-Optima accomplishments in fiscal year 2019 (FY19) focused on prediction of fuel properties and soot formation, as well as ducted fuel injection and biofuel candidates with the potential to reduce particulate matter emissions dramatically, while at the same time lowering nitrogen oxide emissions—suggesting a path to the next generation of high-efficiency, cost-effective, high-performance MCCI engines with decreased emissions-control requirements.

ACI combustion may offer further opportunities to balance engine performance with engine-out emissions for medium- and heavy-duty vehicles. In FY19, this research included exploring the potential of gasoline- and diesel-range fuels, along with advances in engine technologies, to expand stable ACI combustion over a wide speed/load range, controlling engine-out emissions, and ensuring high engine power density. This research is increasing the foundational understanding of fuel properties for advanced combustion modes, including development of new autoignition metrics and use of phi sensitivity as a new fuel property. The heavy-duty ACI research is leveraging current and ongoing findings from the MCCI and light-duty multimode research that have crosscutting applications.

Select Co-Optima accomplishments related to medium- and heavy-duty vehicles are found in the following section.

UPGRADING MYRCENE TO CAMPHORANE PROVIDES A HIGH-CETANE, HIGH-ENERGY MCCI BIOBLENDSTOCK

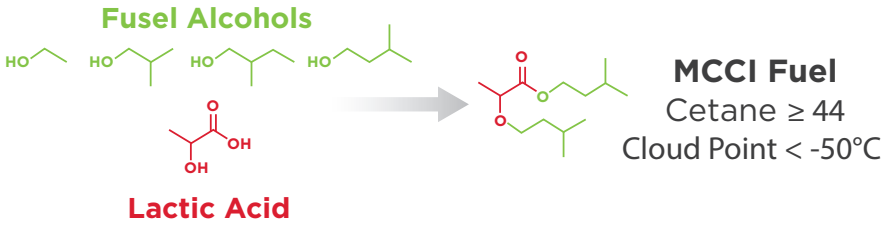
Myrcene is an acyclic monoterpene available from fermentation of sugars or from natural oils. Myrcene contains olefin functional groups, which are easily oxidized and polymerized. In addition, myrcene has a low flash point (44°C), which precludes safe handling, and a low predicted derived cetane number (DCN) of 14, rendering it a poor fuel candidate for use in MCCI engines. However, the olefin functional groups provide access to unique upgrading strategies for high-performance fuel production. In recent work, Co-Optima researchers employed a new approach, upgrading myrcene to the hydrocarbon camphorane via cyclodimerization. This two-step process was accomplished via a thermal Diels-Alder reaction of myrcene and subsequent hydrogenation using an inexpensive nickel-based catalyst with an overall carbon yield above 70%. Camphorane has properties well suited for use as a blendstock in MCCI fuels, including a DCN (57.6) that is 25% higher than that of standard petroleum diesel. Camphorane also has a gravimetric density (0.826 kg/L) close to petroleum diesel's gravimetric density, a flash point high enough for safe handling (115°C), and an energy content nearly identical to that of petroleum diesel (43.23 MJ/kg), suggesting that blending camphorane into petroleum diesel will not reduce fuel economy in diesel vehicles. These properties and the new myrcene-upgrading production pathway make camphorane a promising MCCI bioblendstock candidate. Future work will examine process economics and life-cycle greenhouse gas emissions.



*Comparison of myrcene and camphorane fuel properties in relation to Co-Optima MCCI requirements. LHV = lower heating value; YSI = yield sooting index; * denotes predicted value. Figure by Cameron Moore, LANL*

COMBINING LACTIC ACID AND FUSEL ALCOHOLS RESULTS IN MCCI BIOFUEL WITH HIGH MASS YIELDS

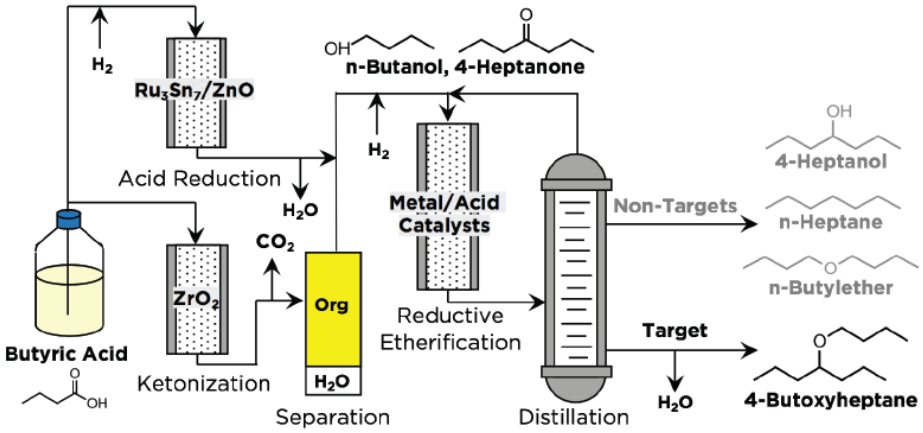
Co-Optima researchers combined two high-yield fermentation products, lactic acid and fusel alcohols, to produce a novel biofuel with properties desirable for use in MCCI engines. Today's highest-volume commercial MCCI biofuel, lipid-based biodiesel, has a limited feedstock resource and can have poor cold-weather performance that limits its use in many regions. Bioderived intermediates and fermentation products can have much lower freezing points but are typically not suitable for MCCI engines or cannot be produced at high rates, yields, and titers. Testing of the novel hydroxyalkanoate-based ether-ester biofuel revealed desirable MCCI properties, such as cetane numbers ranging from 44 to 62, lower heating values >34.5 MJ/kg, and predicted yield sooting indices (YSIs) averaging from 30 to 70. The compound's cloud point (the temperature at which a liquid begins to solidify) of less than −50°C also makes it a viable candidate for cold-weather operation. The combined biological and chemical upgrading pathway used in producing this biofuel converts cellulosic biomass at overall mass yields up to 68% using chemistry similar to that used to produce biodiesel (based on the linear additive theoretical pathway yields of each intermediate). For comparison, the overall mass yield of cellulosic ethanol's production pathway is 45%. Novel fuels produced through this approach from abundant domestic biomass feedstocks may enable the expansion of bioderived alternatives within the diesel fueling infrastructure. Techno-economic analysis (TEA) and life-cycle analysis (LCA) for hydroxyalkanoate-based ether-esters are presented in the highlight, "Economic and Environmental Analyses Provide Metrics to Quickly Gauge Bioblendstock Viability." Future research will examine fuel properties in more detail as well as elastomer compatibility.



High-yield fermentation products that are poor MCCI fuels on their own become desirable MCCI fuels with high cetane, high energy content, and cloud point values below −50 °C. Figure by Joey Carlson, SNL

DIESEL BLENDSTOCK FROM BUTYRIC ACID DEMONSTRATES LOW GREENHOUSE GAS EMISSIONS AND HIGH CETANE NUMBER

Ethers are oxygenated organic compounds that have high cetane numbers and low intrinsic-sooting tendencies, which are desirable properties for diesel fuels. However, the water solubility of many ethers disqualifies them from diesel blending because of concerns about groundwater contamination, as well as the ethers' potential incompatibility with the diesel fueling and engine infrastructure. Co-Optima researchers employed a "fuel-property-first" approach to computationally screen potential ethers for desirable fuel properties before initiating extensive experimental work. The researchers mapped conversion pathways to catalytically upgrade the fermentation product butyric acid into diesel-compatible ethers. They then developed a continuous, solvent-free reductive etherification process to generate the target ether, 4-butoxyheptane. When blended into petroleum-based diesel at 20% by volume, 4-butoxyheptane improved cetane number by 10% and reduced YSI by 20%. Measurements showing low water solubility, relevant polymer compatibility, and storage stability upon adding an antioxidant all demonstrated evidence for safe use within the existing fueling infrastructure. TEA and LCA suggested that, when coupled with adipic acid coproduction from lignin, 4-butoxyheptane could be produced for less than $3 per gasoline gallon equivalent (GGE)—and it could reduce life-cycle greenhouse gas emissions by more than 50% compared to the petroleum diesel it replaces.



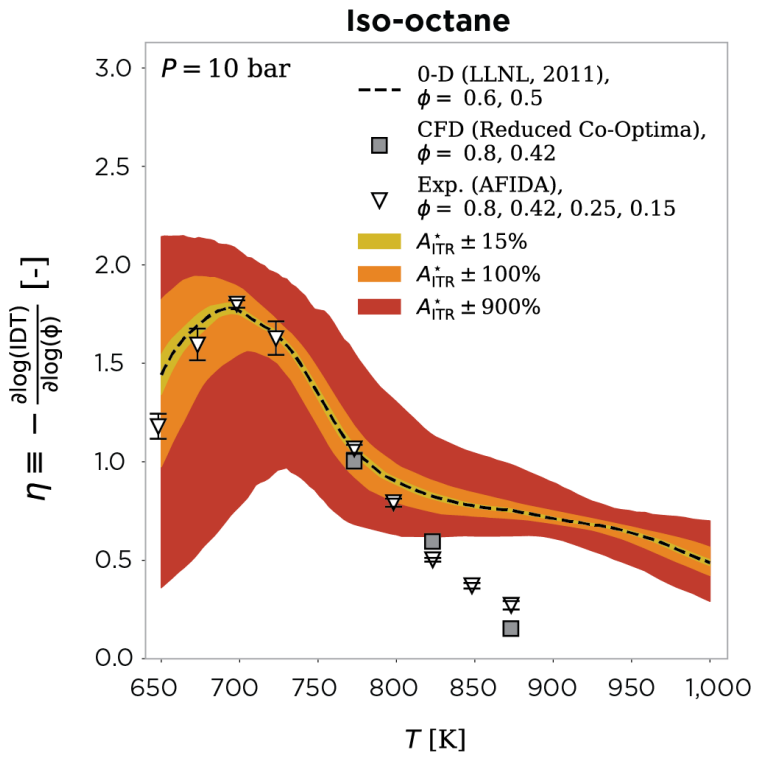
Process design for synthesizing 4-butoxyheptane from butyric acid. Org = organic. Figure by Derek Vardon and Nabila Huq, NREL

MEASUREMENTS AND PREDICTIONS OF IGNITION DELAY TIME AND PHI SENSITIVITY ENHANCE RAPID FUEL SCREENING

Rapid screening of candidate biofuels requires reliable tools for predicting various fuel properties. For advanced compression ignition or multimode engine designs, one such property is phi sensitivity, which represents the change in ignition delay time (IDT) in relation to the fuel-to-air equivalence ratio (phi, or Φ). Co-Optima researchers developed IDT measurement techniques using the Advanced Fuel Ignition Delay Analyzer (AFIDA) to isolate phi-sensitivity effects for a range of fuel-lean conditions (Φ = 0.25–0.80) across engine-relevant pressures and temperatures. In this case, phi sensitivity is defined as

$$\eta \equiv -\frac{d\log(\mathrm{IDT})}{d\log(\phi)};$$

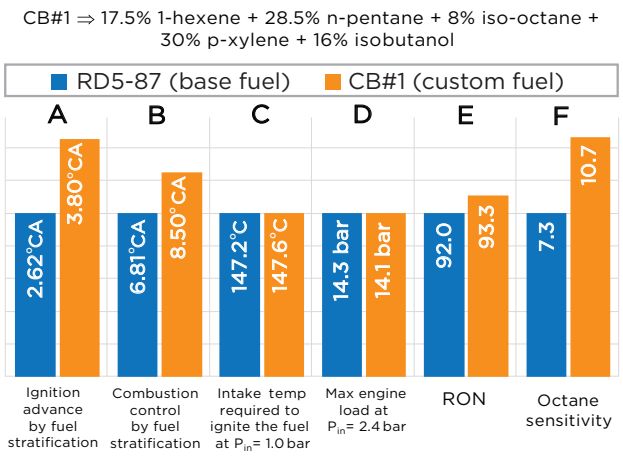
if η were truly only a function of temperature (T) and pressure (P), this proposed log-log definition would be independent of Φ. The researchers also assessed the reliability of existing kinetic reaction mechanisms for iso-octane to predict η by comparing these experimental AFIDA measurements with 0-D (perfectly homogeneous) simulation results. Uncertainties in the 0-D simulations inherited from the underlying reaction mechanism were estimated with neural networks trained to predict phi sensitivity for different intermediate-temperature-reaction (ITR) rate parameters. The 0-D simulations agreed with experimental AFIDA data at low temperatures to within their combined uncertainties of approximately 5%, while computational fluid dynamics (CFD) simulations were required to capture system inhomogeneities at higher temperatures where ignition occurs before mixing is complete (note the poor agreement between experimental η 0-D simulations above 800 K in the figure). The AFIDA-based experiments with small fuel volumes (approximately 150–200 mL) and improved quantitative prediction of phi sensitivity will facilitate both the rapid screening of candidate biofuels for this new fuel property and development of molecular structure relationships to η.



Comparison of phi sensitivity (represented by η) between experimental AFIDA measurements and numerical simulations (0-D and CFD) for iso-octane at fixed P and a range of T. Error bars are 95% confidence intervals for experimental (AFIDA) data. Colors denote 0-D simulation uncertainty corresponding to different levels of uncertainty in the key rate parameters (A_{ITR}). Figure by Richard Messerly and Seonah Kim, NREL

ISOBUTANOL BLEND ENHANCES ACI ENGINE PERFORMANCE

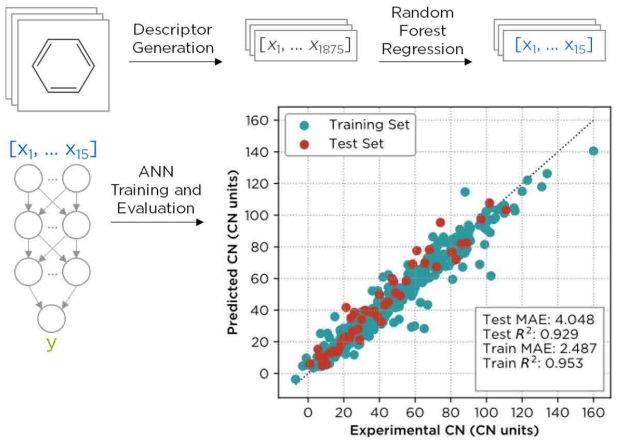
If the fuel is sufficiently phi sensitive, it allows the combustion phasing of an ACI engine to be controlled by varying the charge stratification. This is because regions within the stratified charge that have a higher fuel concentration autoignite faster, advancing the combustion phasing. Phi sensitivity can also provide benefits for increased efficiency, lower noise, and higher loads. Regular gasoline is typically not sufficiently phi sensitive, so Co-Optima researchers computationally designed a gasoline-like isobutanol blend (called CB#1) suitable for ACI and boosted spark-ignition (SI) engines by simultaneously improving phi sensitivity, research octane number (RON), and octane sensitivity. The researchers then experimentally compared CB#1—a five-component, regulation-compliant fuel blend—to RD5-87, a regular E10 (10% ethanol) gasoline. They found that the phi sensitivity of CB#1 was significantly higher than that of RD5-87 (see figure, columns A and B). Similar amounts of intake heat were required to ignite CB#1 and RD5-87 (column C), ensuring that CB#1 can operate in homogeneous charge compression ignition (HCCI) mode as easily as regular gasoline. Similar maximum engine loads were reached with CB#1 and RD5-87 under intake-boosted conditions (column D), but CB#1 provided a higher thermal efficiency at this maximum load. Finally, both RON and octane sensitivity were improved by CB#1 (columns E and F). These results demonstrate that a biofuel blend can be designed to enhance the performance of emerging, highly efficient ACI engines and boosted SI engines.



Experimental results comparing regular E10 gasoline (RD5-87) and a custom-designed blend containing isobutanol (CB#1). Columns A and B are phi-sensitivity metrics; higher values mean the fuel is more phi sensitive. Column C shows the amount of intake heat required to operate in naturally aspirated HCCI mode. Column D shows the maximum engine load achievable under premixed, high-boost HCCI conditions. Columns E and F show the RON and octane sensitivity of the fuels, respectively. CA = crank angle. Figure by Dario Lopez-Pintor, SNL

ARTIFICIAL NEURAL NETWORKS PREDICT FUEL PROPERTIES WITH 96% ACCURACY, ENABLE RAPID BIOFUEL SCREENING

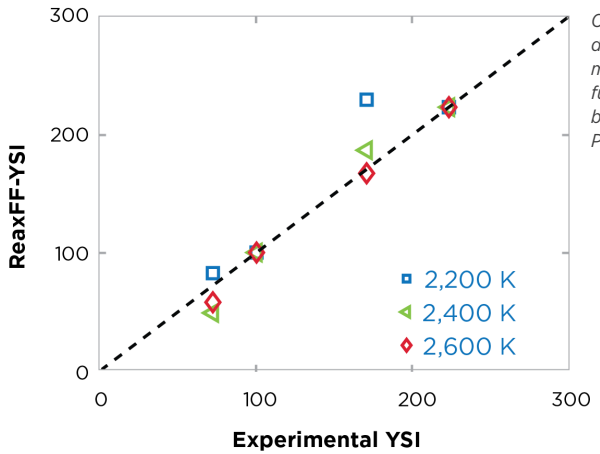
Computational models trained to predict key fuel properties provide researchers with rapid screening tools for alternative fuel development. Co-Optima researchers employed artificial neural networks (ANNs) to construct predictive models for cetane number (CN), yield sooting index, research octane number, motor octane number, kinematic viscosity, pour point, and cloud point. Each model predicted property values with greater than 96% accuracy for compounds outside the training set. The researchers then improved the models using optimization algorithms—based on the behavior of artificial bee colonies—to tune ANN hyperparameters applicable to the training process. The artificial bee colony method is well suited to the dimensionality of ANN hyperparameter problems, in which the solution search space is in as many dimensions as the number of parameters being tuned, as is the case for honeybee foraging techniques. This is the first application of this new method, a mathematical attempt to replicate a natural process that has evolved over a long period, to molecular property networks. The inclusion of hyperparameter tuning provided (on average) a 20.4% reduction in the model's mean absolute error (MAE). The improved model performance was used by the researchers to preemptively screen compounds that result from fast pyrolysis and catalytic upgrading of lignocellulosic biomass, ultimately providing insight into which renewable products are likely to perform optimally in target engine architectures. The open-access property-prediction (ECNet) and optimization (ECabc) platforms are available on GitHub for community use at https://github.com/ECRL.



Workflow illustrating quantitative structure-property relationships (QSPR) descriptor generation, descriptor selection via random forest regression, ANN training, and evaluation of the model for a particular property (CN). Figure by John Hunter Mack and Travis Kessler, University of Massachusetts Lowell

MOLECULAR DYNAMICS SIMULATIONS ENABLE PREDICTION OF BIOFUEL SOOTING TENDENCIES

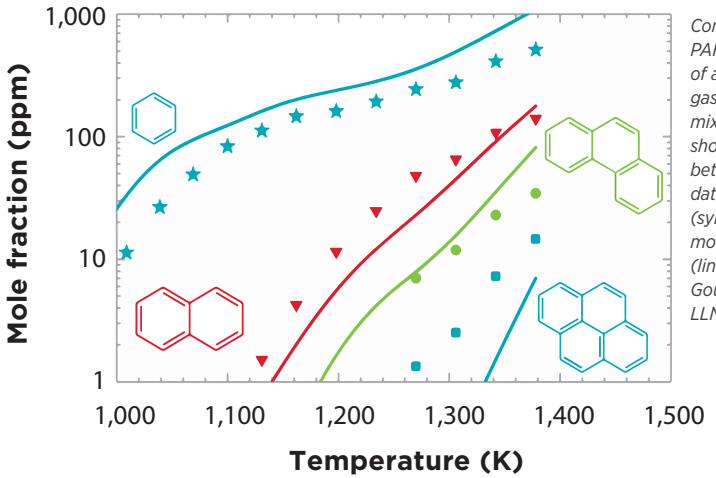
Co-Optima uses simulation tools to predict the amount of soot that a new biofuel would produce during combustion. However, these tools generally require experimentally derived knowledge of chemical mechanisms or functional groups. To overcome this limitation, Co-Optima researchers used the ReaxFF reactive molecular dynamics software to analyze fuel-consumption pathways and soot-formation pathways and, ultimately, to predict the sooting tendency of fuels based on molecular structure alone. The ReaxFF simulations predict YSI by solving the equations of motion for an ensemble of fuel molecules with empirical force fields around each atom. The researchers validated this approach using the well-characterized fuels toluene and phenol, for which the reaction pathways occurring in the ReaxFF simulations are consistent with the present chemical-kinetic understanding. Currently, the researchers are applying the ReaxFF framework to molecules with chemical kinetics that are poorly understood, such as oxygen-containing aromatic compounds like guaiacol and syringol, which can be derived from lignin. In addition, the researchers are using this approach to estimate YSIs for fuels that are potentially promising candidates but difficult to synthesize, such as those containing strained cyclopropyl rings. Sooting tendencies have been calculated for hexylamines as well, demonstrating the wide applicability of this approach. This work could also be adapted to predict properties beyond YSI. These enhanced predictive capabilities have potential to accelerate the identification and development of biofuels with desirable properties.



Correlation between ReaxFF-derived and experimentally measured YSIs for the reference fuels ethylbenzene and benzene. Figure by Yuan Xuan, Pennsylvania State University

MODEL SIMULATES FORMATION OF PAHS AND PREDICTS THEIR CONTRIBUTION TO SOOTING

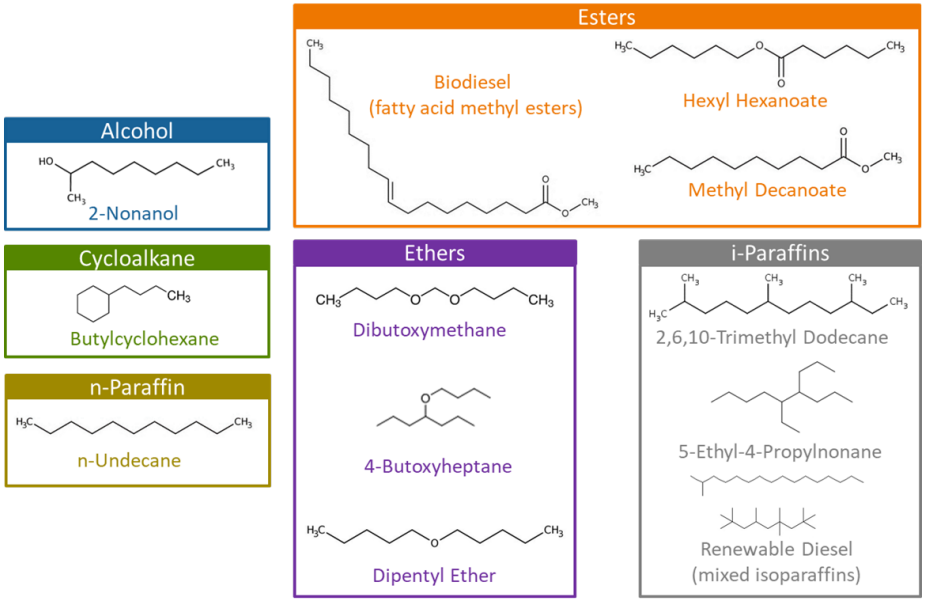
Accurate particulate matter (PM) formation models must be integrated with engine simulations to predict the effects of fuel composition on PM emissions. However, developing a kinetic model that accurately predicts concentrations of polycyclic aromatic hydrocarbons (PAHs)—soot precursors that form during combustion—has been a longstanding challenge for the combustion research community. Co-Optima researchers helped fill this gap by incorporating recently available PAH-formation reaction rates and product channels into a new PAH model, which also captures formation of PAHs from aromatic components already present in the fuel. The researchers validated the model for PAH sizes up to seven rings by comparing experimental results to simulated results for the pyrolysis of acetylene, ethylene, propene, cyclopentene, cyclopentadiene, n-dodecane, and a three-component gasoline surrogate mixture (n-heptane/iso-octane/toluene). Overall, the experimental and simulated results show significantly improved agreement relative to prior simulations. The researchers also linked this PAH model to a soot sectional model that enables comparison of preliminary soot predictions with measured soot data from fundamental combustion devices. This is a significant step toward an improved soot-prediction submodel for use in multidimensional engine simulations.



Concentrations of major PAHs during pyrolysis of a three-component gasoline surrogate mixture in a flow reactor, showing agreement between experimental data from the literature (symbols) and PAH model predictions (lines). Figure by Goutham Kukkadapu, LLNL

BIOFUEL CANDIDATES SHOW PROMISE FOR REDUCING DIESEL ENGINE PARTICULATE MATTER EMISSIONS

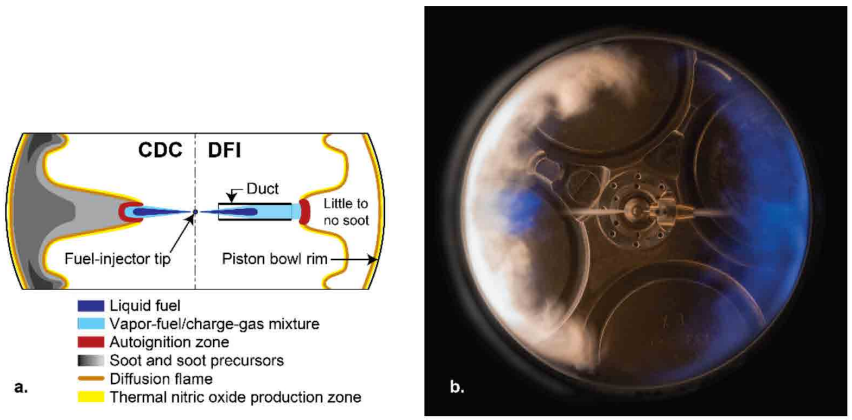
Diesel MCCI engines are highly efficient and likely will continue to dominate cargo transportation for years to come. To help harness the efficiency benefits of MCCI engines while mitigating their impacts, Co-Optima researchers identified biofuel candidates with potential to reduce net carbon and other pollutant emissions as replacements for petroleum-based diesel fuel. Researchers used the Co-Optima Fuel Properties Database and fuel-property predictive tools to identify candidate molecules spanning a wide range of functional groups, such as alcohols, hydrocarbons, esters, and ethers. Assessment of promising candidates included measuring pure-component and blended-fuel properties. All the candidates showed potential for successful blending in commercial diesel fuel. In addition, all of them demonstrated yield sooting index values lower than those of conventional diesel fuel, with several providing an almost 50% reduction. For this reason, they may be capable of reducing particulate matter emissions in diesel engines, while also providing the sustainability and environmental benefits of low-net-carbon biofuels. Many of these candidates are currently being examined in engine combustion experiments.



Chemical structures of MCCI biofuel candidates meeting the property requirements for blending into conventional diesel. Figure by Gina Fioroni, NREL

COMBINATION OF DFI WITH OXYGENATED FUEL INDICATES PROMISING PATH FOR FUTURE ENGINES AND FUELS

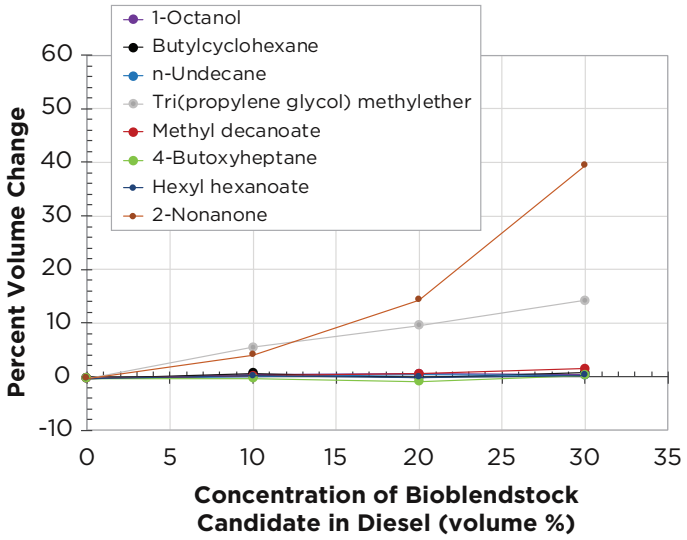
Ducted fuel injection (DFI) involves injecting fuel along the axis of one or more small tubes installed within the combustion chamber of a diesel engine. As in a Bunsen burner, each tube facilitates premixing of the fuel and oxidizer before ignition, dramatically curtailing or even preventing soot formation. Soot emissions are attenuated even under dilute (i.e., low-oxygen) conditions that also produce low emissions of nitrogen oxides (NO_x). Hence, DFI has been shown to enable simultaneously low soot and NO_x emissions, removing the primary barrier to the broader deployment of high-efficiency diesel engines. In addition, DFI is synergistic with potential renewable, oxygenated fuels. Research in FY19 showed not only that DFI lowers in-cylinder soot incandescence by ~90% with conventional diesel fuel, but also that changing to a fuel containing 25% by volume of a renewable, oxygenated blendstock leads to an additional ~90% in-cylinder soot incandescence reduction under low-NO_x conditions. This could significantly lower the costs of exhaust-gas aftertreatment systems required to ensure compliance with emissions regulations while providing an economic incentive for using sustainable fuels. Finally, DFI is conceivably retrofittable into existing diesel engines, potentially enabling rapid emissions reductions without requiring complete engine replacements.



Conventional diesel combustion (CDC) vs. DFI. (a.) Schematic showing a CDC spray on the left side of the combustion chamber and a DFI spray on the right. (b.) Color picture of the combustion event depicted in the schematic. The whitish crescent on the left (CDC) side is produced by incandescence from hot soot. The crescent on the right (DFI) side is blue because there is no soot formed. Figure by C.J. Mueller, SNL

STUDIES INDICATE COMPATIBILITY OF MCCI BLENDSTOCK CANDIDATES WITH FUEL SYSTEM COMPONENT MATERIALS

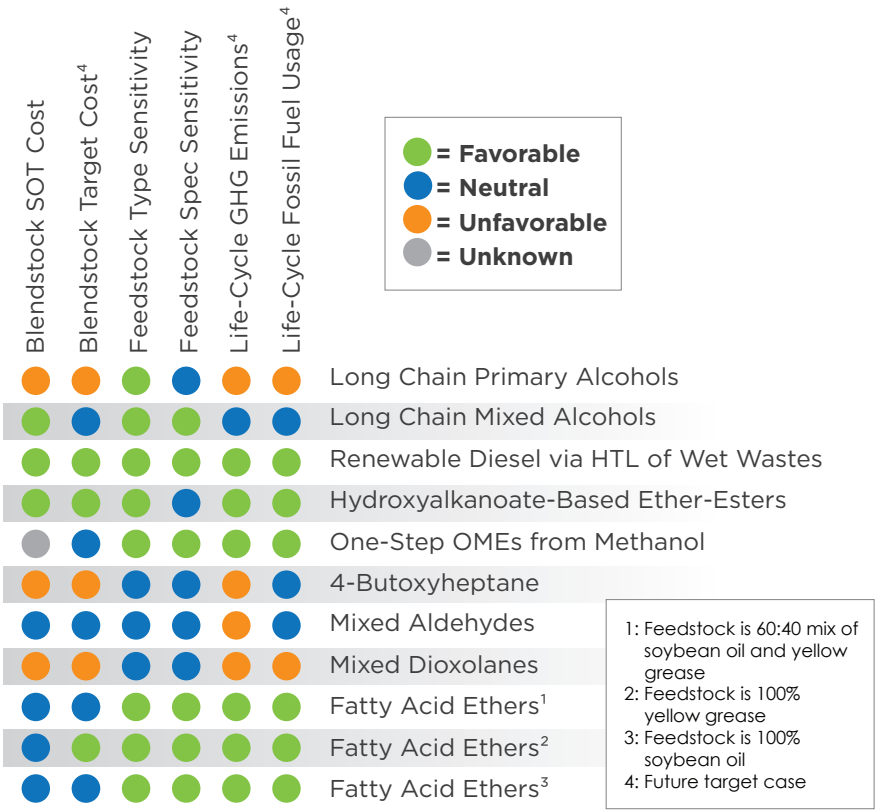
Elastomer materials are critical components of fuel system seals and hoses. If a fuel causes component materials to swell excessively, the materials may lose structural integrity, resulting in leakage or—in dynamic applications such as valves—the seizing up of moving parts. Co-Optima exposure studies showed strong compatibility for six of eight MCCI blendstock candidates with fueling-infrastructure elastomers, including acrylonitrile rubbers, fluorocarbons, fluorosilicone, neoprene, and epichlorohydrin rubber. The eight blendstocks were blended with diesel at levels of 10%, 20%, and 30% by volume. The compatibility threshold for elastomer volume expansion of less than 15% was met by 1-octanol, n-undecane, methyl decanoate, hexyl hexanoate, butylcyclohexane, and 4-butoxyheptane. However, blends containing tripropylene glycol methylether and 2-nonanone were markedly less compatible with the elastomers studied and would not be deemed suitable for some sealing applications. These results highlight the need for exposure-based compatibility studies to ensure blendstock candidates are compatible with existing materials.



Percent volume change of fluorocarbon elastomer vs. concentration of blendstock candidates in diesel. Fluorocarbons are used extensively in fuel storage and dispensing systems, and in onboard vehicle fueling systems. Figure by Mike Kass, ORNL

ECONOMIC AND ENVIRONMENTAL ANALYSES PROVIDE METRICS TO QUICKLY GAUGE BIOBLENDSTOCK VIABILITY

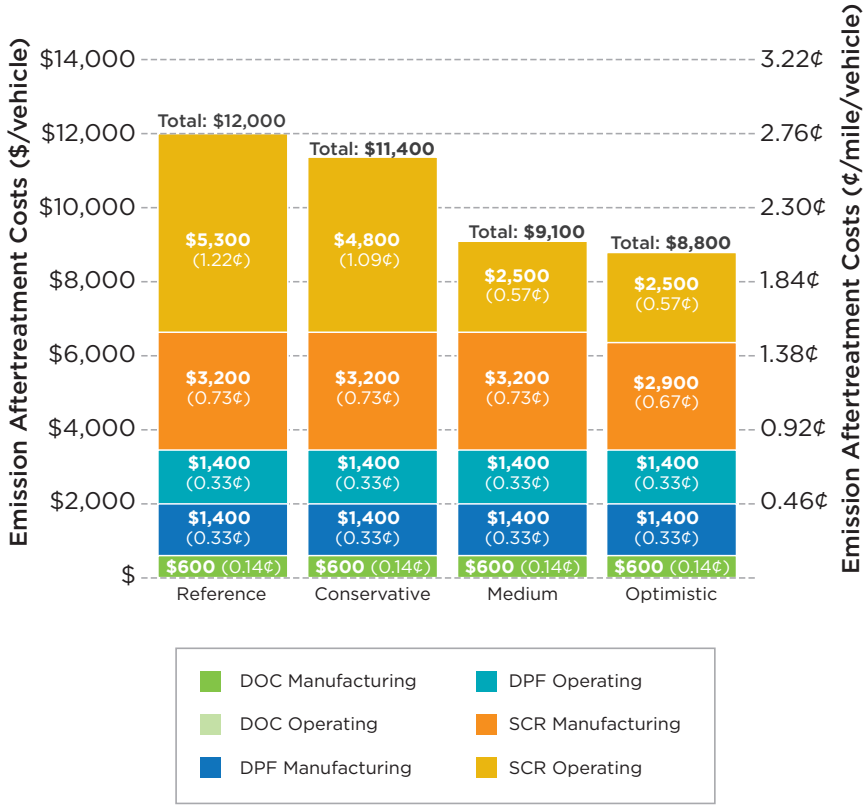
Economic and environmental benefits are vital considerations for large-scale development and deployment of sustainable fuels. Researchers assessed 11 emerging pathways that will enable the production of Co-Optima MCCI bioblendstocks. TEA and LCA were used to evaluate technological readiness, economic and process feasibility, and sustainability metrics. Benchmarking against current state of technology (SOT), the three most favorable pathways (renewable diesel via HTL of wet wastes, hydroxyalkanoate-based ether-esters, and fatty acid ethers from yellow grease) showed an estimated minimum fuel-selling price at or below $5/GGE, while future targeted technological advancements offer the potential for further lowering the price to $4/GGE or less. Most of the conversion technologies are robust, with fuel yield and quality minimally affected by changing the feedstock type (such as from one biomass type to another) or changing feedstock specifications (such as moisture content or slight variations in composition). However, ongoing research is needed to help fill knowledge gaps related to the blending behavior of these bioblendstocks with existing fuels, and further testing is required to understand how much can be blended while still meeting legal specifications. In addition, because all feedstocks may be limited in total or regional supply, feedstock resource availability is an important consideration that is currently being explored in other Co-Optima projects. Most of the MCCI bioblendstocks showed significant reductions in life-cycle greenhouse gas (GHG) emissions and fossil energy consumption relative to conventional diesel fuel, with more than half demonstrating a reduction greater than 60% for both metrics. Results from these analyses provide metric ranges to enable researchers and industry to quickly gauge economic and environmental favorability across a wide range of bioblendstocks.



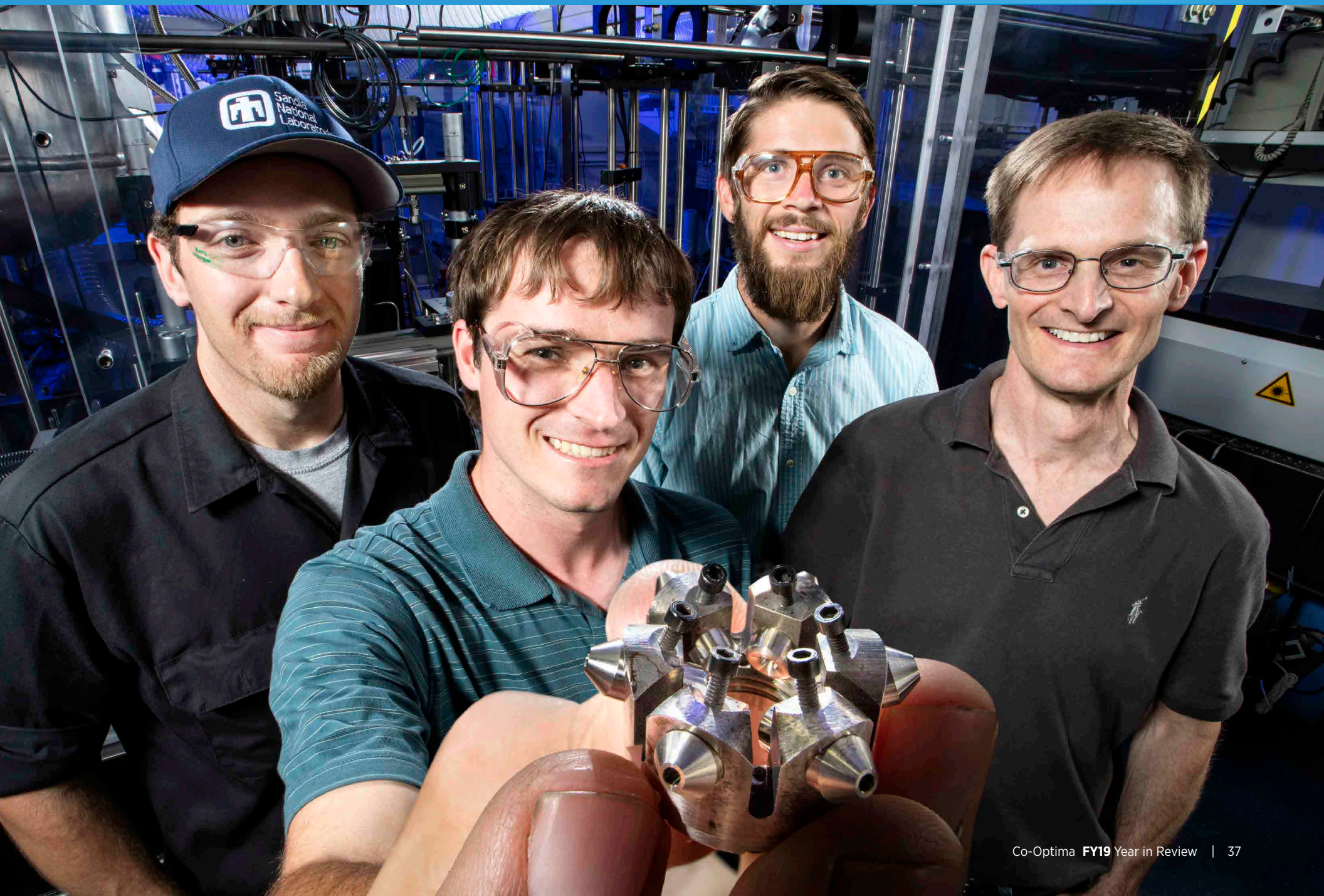
Comparison matrix for a selected subset of TEA and LCA results for the 11 evaluated Co-Optima MCCI bioblendstock pathways. Results are categorized and compared based on favorability for each metric. Routes produced biochemically do not include the valorization of lignin to coproducts. Additional information on hydroxyalkanoate-based ether-esters and 4-butoxyheptane can be found in other highlights. HTL = hydrothermal liquefaction; OME = oxymethylene dimethyl ether. Figure by Andrew Bartling, NREL

MCCI CO-OPTIMIZATION COULD REDUCE HEAVY-DUTY VEHICLE EMISSIONS AND AFTERTREATMENT COSTS

The MCCI engines used in today's heavy-duty vehicles are subject to stringent emissions regulations that necessitate expensive aftertreatment systems. Reducing engine-out emissions by co-optimizing MCCI engines and biofuel blends could lower the capital and operating costs of required aftertreatment devices while increasing the renewable content of diesel fuels. Based on input from engine and aftertreatment experts, Co-Optima researchers quantified aftertreatment capital and operating costs in vehicles with MCCI engines. They applied these costs to four scenarios for Class 8 long-haul tractor-trailers, with the reference scenario representing current MCCI engine technology and diesel fuel with corresponding aftertreatment. Compared with the reference scenario, co-optimization of MCCI engines and fuels saves $600 (0.14¢/mile) in aftertreatment costs over the lifetime of the vehicle in a conservative scenario in which engine-out emissions of NO_x and PM are reduced by 10%. The savings rise to $2,900 (0.67¢/mile) in a medium scenario in which the emissions are reduced by 50%. In an optimistic scenario, reducing the emissions by 50% while downsizing the selective catalytic reduction (SCR) device by 15% saves $3,200 (0.74¢/mile). The largest proportion of savings stems from the decreased SCR operating costs enabled by the lower engine-out NO_x emissions (reduced diesel exhaust fluid consumption). The estimated savings are likely sufficient to motivate continued research on reducing pollutant emissions via MCCI co-optimization. Even larger benefits may be possible for heavy-duty vehicles that experience more frequent stop-and-go operation.



Lifetime capital (manufacturing) and operating costs per vehicle and per mile in the reference, conservative, medium, and optimistic scenarios. DOC = diesel oxidation catalyst; DPF = diesel particulate filter. Figure by Hao Cai, ANL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NEXT STEPS

The Co-Optima team will continue to push the boundaries of light-duty engine efficiency and fuel economy by focusing on multimode combustion approaches. Medium- and heavy-duty research will further explore new low-net-carbon blendstocks and the potential of ducted fuel injection for mixing-controlled compression ignition (MCCI) combustion along with new opportunities for advanced compression ignition (ACI) combustion. Specific areas will include the following:

- Improve fundamental understandings of the impacts of fuel characteristics and engine parameters on light-duty multimode combustion performance, including defining important fuel properties and target property values
- Identify blendstocks with fuel properties that enable highly efficient light-duty multimode combustion
- Perform techno-economic analysis (TEA), life-cycle analysis (LCA), and refinery benefits analysis for multimode blendstocks
- Identify and characterize MCCI blendstocks that provide key fuel properties for manipulating the tradeoff between particulate matter and nitrogen oxides emissions, enabling new opportunities for reducing engine-out emissions
- Complete and report TEA, LCA, and refinery benefits analysis for candidate MCCI blendstocks
- Define important fuel properties and target property values for medium- and heavy-duty ACI combustion
- Continue expanding our understanding of molecular structure effects on fuel properties, mixing, soot formation, and autoignition.

Co-Optima will continue focusing on foundational science and delivering objective scientific outcomes necessary for informed decision making to American industry and policymakers.

PUBLICLY AVAILABLE TOOLS AND DATA

Many Co-Optima accomplishments have been made possible by the team's development of new capabilities, numerical algorithms, and computational tools. The following data and tools can be accessed online by the wider research community.

Fuel Properties Database
www.nrel.gov/transportation/fuels-properties-database

The continuously updated Fuel Properties Database focuses on biobased fuel blendstocks (both pure components and mixtures) under investigation by the Co-Optima team and is populated with data from literature, as well as measured and/or predicted data. It contains data on more than 400 biobased fuel blendstocks, as well as on gasoline and gasoline surrogates designed for such blending.

RetSynth Tool
https://github.com/sandialabs/RetSynth

The RetSynth (retrosynthesis) tool can be used to rapidly identify and evaluate the viability of pathways for producing biobased 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, including 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.

Yield Sooting Index Tool
https://ysipred.herokuapp.com

Researchers integrated the yield sooting index (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.

Co-Optimizer Tool
https://github.com/NREL/cooptima-co-optimizer

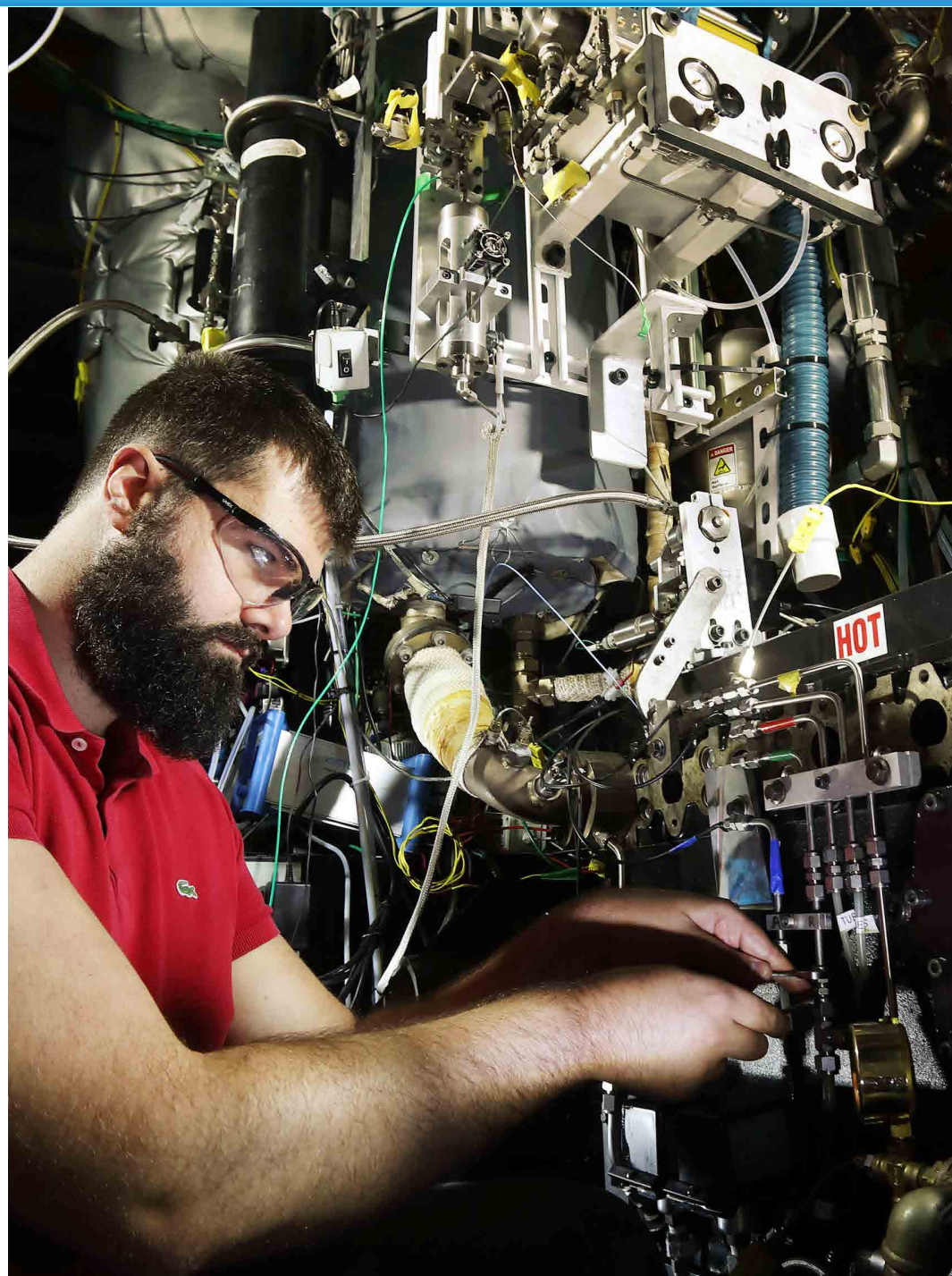
The Co-Optimizer software tool makes it possible to assess candidate blendstocks in relation to tradeoffs involving a number of complex variables, including production scale and economics, life-cycle emissions, and infrastructure compatibility. Using the Co-Optima boosted spark-ignition merit function to identify blendstocks with the requisite properties to maximize engine efficiency when blended into petroleum base fuels, the tool uses Co-Optima-developed blending models to identify fully blended fuels that meet current fuel-quality specifications. User-supplied constraints then identify a smaller subset of solutions that can be compared over a wide range of market-introduction scenarios.

ECNet Tool
https://github.com/ECRL/ECNet

ECNet is a machine-learning framework for predicting a variety of fuel properties, including cetane number and YSI, based on molecular structure and using artificial neural networks. Precompiled databases for each of the properties are ready for use, and extensive documentation outlining how to construct the models is available. Developers continually add software enhancements to reduce the time required to construct models while increasing model accuracy.

PUBLICATIONS AND MEDIA COVERAGE

Co-Optima researchers have continued their strong scientific publication track record, with more than 30 peer-reviewed journal articles and peer-reviewed conference papers published during fiscal year 2019 (FY19). A new publications database has been made available online (https://www.energy.gov/eere/bioenergy/co-optima-publications-library-0) and currently has more than 150 entries. In FY19, especially notable publications include the "Top 10 Report," which describes an assessment of 400 biofuel-derived molecules and identifies the top candidates to blend with petroleum fuel to increase boosted spark-ignition engine efficiency. In addition, Co-Optima researchers contributed to a study of high-octane ketone production published in *Nature Communications*. Beyond the publications developed by Co-Optima participants, various Co-Optima activities were covered by trade and popular media outlets in FY19.



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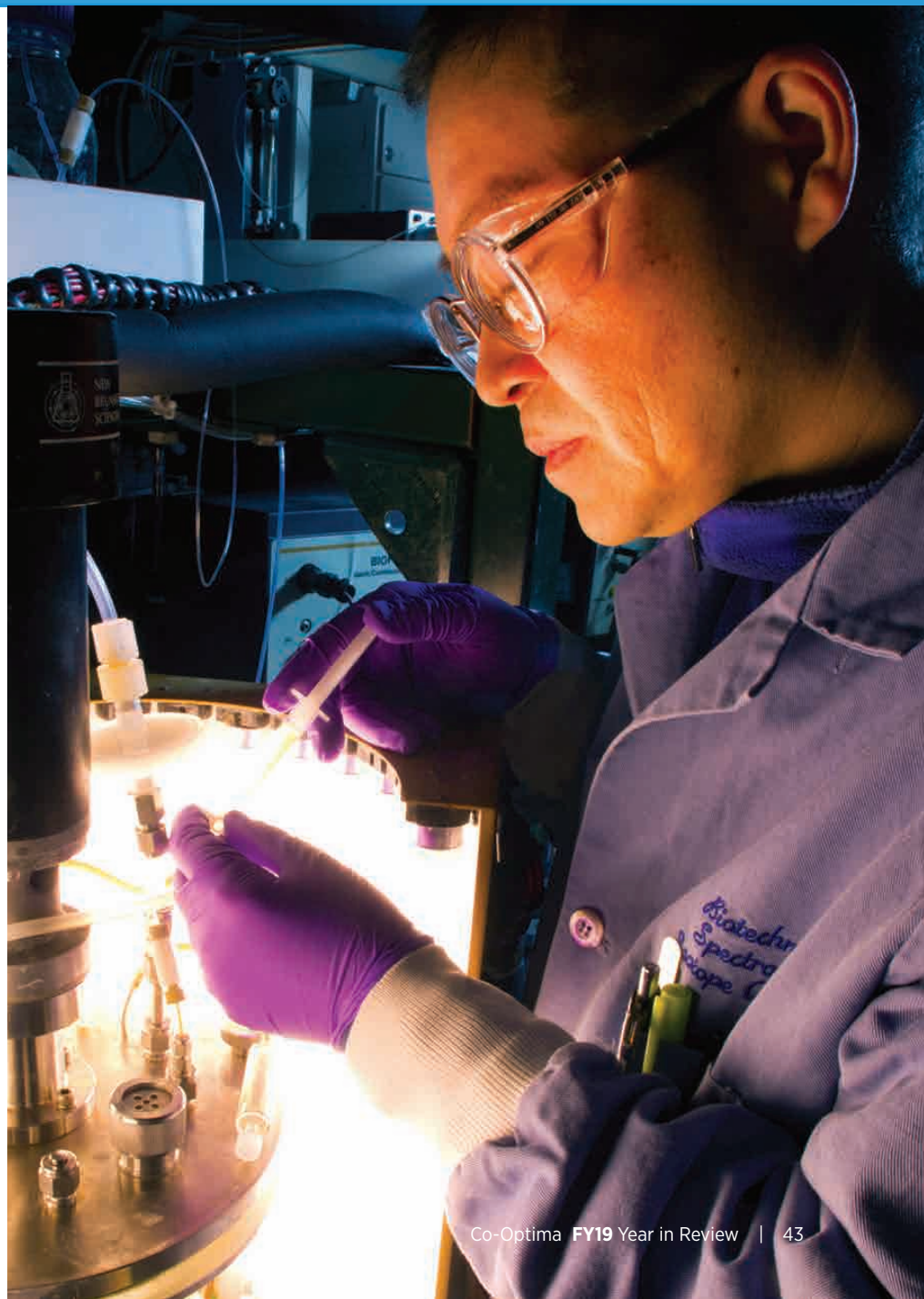

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ACRONYMS AND ABBREVIATIONS

ABLC ..... Advanced Bioeconomy Leadership Conference

ACI ..... advanced compression ignition

ADOPT ..... Automotive Deployment Options Projection Tool

AFIDA ..... Advanced Fuel Ignition Delay Analyzer

AKI ..... anti-knock index

ANL ..... Argonne National Laboratory

ANN ..... artificial neural network

aTDC ..... after top dead center

BDC ..... bottom dead center

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

Bioeconomy AGE ..... Bioeconomy Air Emissions, Greenhouse Gas Emissions, and Energy Consumption

BOB ..... blendstock for oxygenate blending

BSFC ..... brake-specific fuel consumption

BSM ..... Biomass Scenario Model

CA ..... crank angle

CA50 ..... crank angle at which 50% of the fuel has burned

CAD ..... crank angle degree

CARBOB ..... California Reformulated blendstock for oxygenate blending

CDC ..... conventional diesel combustion

CFD ..... computational fluid dynamics

CFR ..... Cooperative Fuels Research

CN ..... cetane number

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

CPA ..... Cubic-Plus-Association

CR ..... compression ratio

DCN ..... derived cetane number

DFI ..... ducted fuel injection

DIB ..... diisobutylene

DISI ..... direct-injection spark ignition

DMF ..... dimethylfuran

DOC ..... diesel oxidation catalyst

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

DPF ..... diesel particulate filter

E0 ..... gasoline containing 0% ethanol

E10 ..... gasoline containing 10% ethanol

E15 ..... gasoline containing 15% ethanol

E22 ..... gasoline containing 22% ethanol

E30 ..... gasoline containing 30% ethanol

EEE ..... emissions certification fuel

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

EtOH ..... ethanol

FACE ..... Fuels for Advanced Combustion Engines

FSC ..... Fuel Science Center

FY ..... fiscal year

GGE ..... gasoline gallon equivalent

GHG ..... greenhouse gas

GREET ..... Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation

HCCI ..... homogeneous charge compression ignition

HOV ..... heat of vaporization

HTL ..... hydrothermal liquefaction

iBuOH ..... isobutanol

IDT ..... ignition delay time

iPrOH ..... isopropanol

ITE ..... indicated thermal efficiency

ITHR ..... intermediate-temperature heat release

ITR..... intermediate-temperature reaction

KLSA ..... knock-limited spark advance

LANL..... Los Alamos National Laboratory

LBNL ..... Lawrence Berkeley National Laboratory

LBV ..... laminar burning velocity

LCA..... life-cycle analysis

LD..... light duty

LFS..... laminar flame speed

LHV..... lower heating value

LLNL..... Lawrence Livermore National Laboratory

LP ..... linear programming

LTHR..... low-temperature heat release

MAE..... mean absolute error

MCCI..... mixing-controlled compression ignition

MCP ..... methylcyclopentane

MON ..... motor octane number

NO_x..... nitrogen oxides

NREL..... National Renewable Energy Laboratory

NRTL..... nonrandom two-liquid activity coefficient model

NUIG..... National University of Ireland Galway

OI..... octane index

OME..... oxymethylene dimethyl ether

ORNL ..... Oak Ridge National Laboratory

P..... pressure

PAH..... polycyclic aromatic hydrocarbon

Pc ..... compressed pressure

PM ..... particulate matter

PMI..... particulate matter index

PNNL..... Pacific Northwest National Laboratory

PRF ..... primary reference fuel

QSPR..... quantitative structure-property relationship

RCM..... rapid-compression machine

RMG..... Reaction Mechanism Generator

RMSE..... root-mean-square error

RON..... research octane number

RVP..... Reid vapor pressure

S..... octane sensitivity

SACI..... spark-assisted compression ignition

SCR..... selective catalytic reduction

SI..... spark ignition

SNL ..... Sandia National Laboratories

SOT..... state of technology

ST ..... spark timing

T..... temperature

Tc..... compressed temperature

TEA..... techno-economic analysis

TG..... Co-Optima test gasolines

THF ..... tetrahydrofuran

TSF..... toluene standardization fuel

UDDS ..... Urban Dynamometer Driving Schedule

UNIFAC ..... UNIQUAC (universal quasichemical) Functional-Group Activity Coefficients

UNIF-DMD..... UNIFAC with Dortmund modification

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)

direct-injection spark ignition (DISI) ..... 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, coaxial 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

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

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 offices under the U.S. Department of Energy (DOE) Office of Energy Efficiency & Renewable Energy (EERE) and nine National Laboratories, Co-Optima has one industry-led and 17 university-led research projects, with numerous additional university and industry partners. Co-Optima has engaged with representatives from other government agencies, the petroleum and biofuels industries, automakers, and trade and consumer groups. In fiscal year 2019 (FY19), several new projects were awarded, and additional universities and industry groups were integrated into the Co-Optima team.

The Co-Optima team had two unique opportunities to engage with international researchers and industry in FY19. In May 2018, several team members traveled to Germany's RWTH Aachen University to present an update on the Co-Optima initiative at the Fuel Science Center (FSC) Annual Conference, and to explore potential synergies between Co-Optima and the FSC. The FSC is a newly awarded center, analogous to Co-Optima, that builds on the success of the RWTH Aachen University-led "Tailor-Made Fuels from Biomass" Cluster of Excellence. In July 2018, Co-Optima representatives and DOE leadership traveled to Japan to foster discussion and share information about engine and fuels research, meeting with Honda, Toyota, Nissan, Denso, Mazda, Isuzu, and Hino. This was a unique opportunity to understand the status of engine and fuels research in Japan.

Co-Optima team members regularly present at conferences and are active participants in professional societies. In FY19, these forums included the Advanced Bioeconomy Leadership Conference (ABLC), ABLC NEXT, SAE World Congress, SAE Powertrain Fuels and Lubricants Meeting, SAE Innovations in Mobility Conference, Transportation Research Board Annual Meeting, FSC Annual Conference, International Energy Agency Combustion Task Leaders Meeting, and American Chemical Society National Meeting. In addition, the Co-Optima team had five presentations at the biannual Bioenergy Technologies Office Peer Review, 12 presentations at the Vehicle Technologies Office Annual Merit Review, and numerous additional presentations at universities and for a range of stakeholders.

These exchanges have helped pinpoint research and development 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 Laboratories and EERE recognize that continued exchanges with these partners help focus and prioritize Co-Optima research and development on areas with the greatest chance for near-term market impact and are vital to the ongoing success of the initiative.

energy.gov/fuel-engine-co-optimization

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