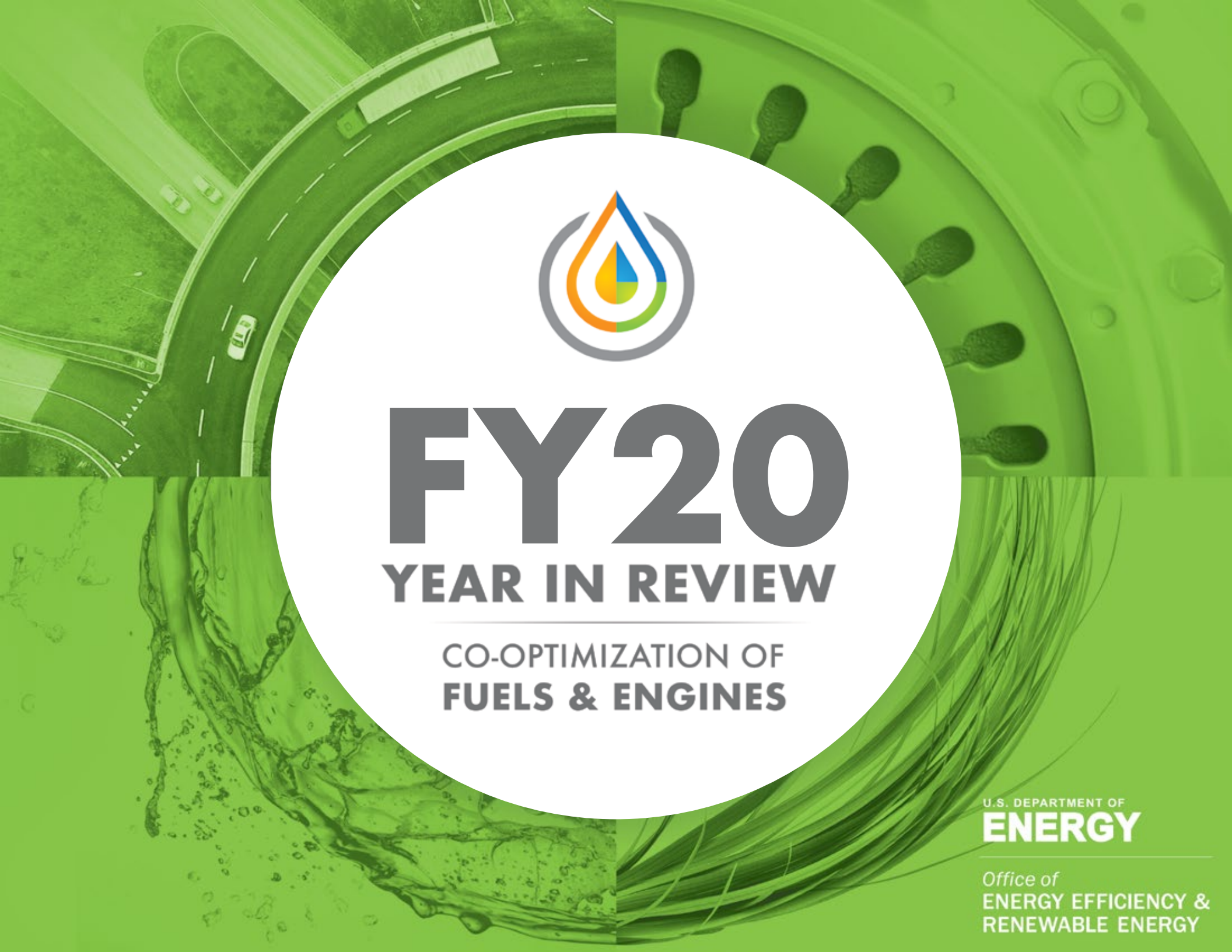

FY20
YEAR IN REVIEW

CO-OPTIMIZATION OF FUELS & ENGINES

U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

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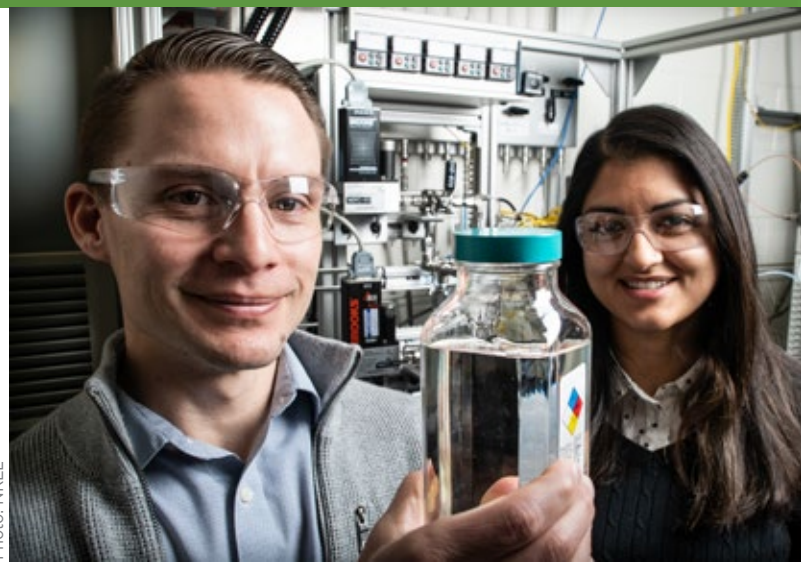

Photo: NREL

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 vehicle 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 35 industry and university partners. This initiative is targeting solutions with potential to improve gasoline and diesel fuels and engines in the marketplace today, as well as solutions that could lead to revolutionary technologies for the vehicles of tomorrow.

PREFACE: SUSTAINING MOMENTUM IN CHALLENGING TIMES

Internal combustion engines and liquid fuels will continue to dominate transportation for many years. This reality—coupled with a global push to maximize energy efficiency, increase the use of renewable resources, and decrease transportation sector emissions—has continued to spur significant interest in the Co-Optimization of Fuels & Engines (Co-Optima) initiative and reinforces the urgency of our research. Our scientists, engineers, and analysts are working with other experts from across the country to give industry, policy, and research decision makers the knowledge, data, and tools they need to identify the most viable and beneficial combinations of high-performance fuels and engines for American drivers, businesses, and the environment.

Fiscal Year 2020 (FY20) was a productive and challenging year for the Co-Optima team. Extending our foundation of science and knowledge to simultaneously improve the performance of fuels and engines for light-duty (LD), medium-duty (MD), and heavy-duty (HD) vehicles, accomplishments included:

- Co-Optima researchers determined target fuel properties for three LD multimode combustion approaches that combine spark ignition (SI), advanced compression ignition (ACI), and other strategies to maximize efficiency and minimize emissions.
- The evaluation of 14 potential mixing-controlled compression ignition (MCCI) blendstocks revealed strong potential for most to meet production and operational cost requirements, while seven demonstrated the ability to cut life cycle greenhouse gas (GHG) emissions by more than 60% in comparison to conventional petroleum-derived diesel.
- Numerous peer-reviewed journals published articles on Co-Optima findings, with the team producing more than 60 reports, papers, and other publications.
- Through a competitive process, the U.S. Department of Energy (DOE) selected seven industry-led projects to accelerate the development and adoption of commercial high-performance biofuels by leveraging the unique experimental and computational capabilities of the National Laboratories.

More detail on these and other significant LD, MD, and HD accomplishments can be found throughout this report. Summaries of four high-impact publications, along with a more comprehensive list of this year's Co-Optima publications, can be found at the end of this report.

Photo: LBNL

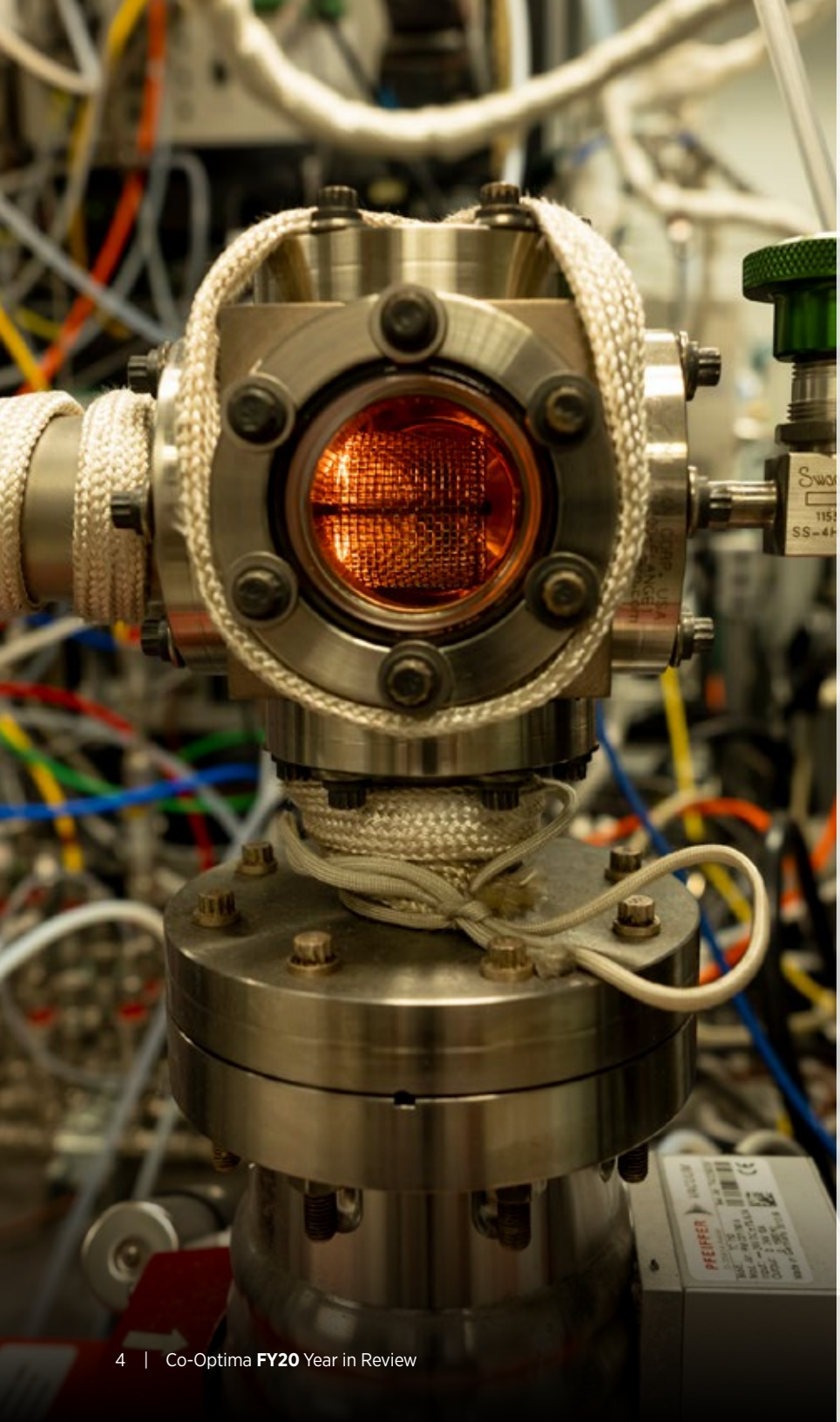

Photo: ORNL

As was the case the world over, our FY20 was also dominated by challenges related to the COVID-19 pandemic. Concerns about personal health and safety translated into the elimination of in-person collaborations and reduced access to experimental facilities. Rapid shutdowns in the spring quickly brought all face-to-face meetings to a halt, including our annual all-hands meeting, which was originally scheduled for the week in March when much travel in the United States came to a halt.

The team continues to adapt to ever-changing conditions, ensuring that the science perseveres—even as many of us juggle these responsibilities with demands including children's remote learning and caregiving for those affected by the illness. With our team already spread out across the country, and thanks to the collaborative spirit that has been a hallmark of the Co-Optima initiative from the beginning, we seamlessly shifted to enhance our capabilities for virtual engagement, with record attendance at our online all-hands meeting and uninterrupted momentum in our research.

At the end of FY20, we continue our transition to more focus on MD/HD research. 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 the vision and support that have enabled the success of this initiative. We also thank our external advisory board for the continued guidance that has been critical to ensuring the value of this initiative to American industry.

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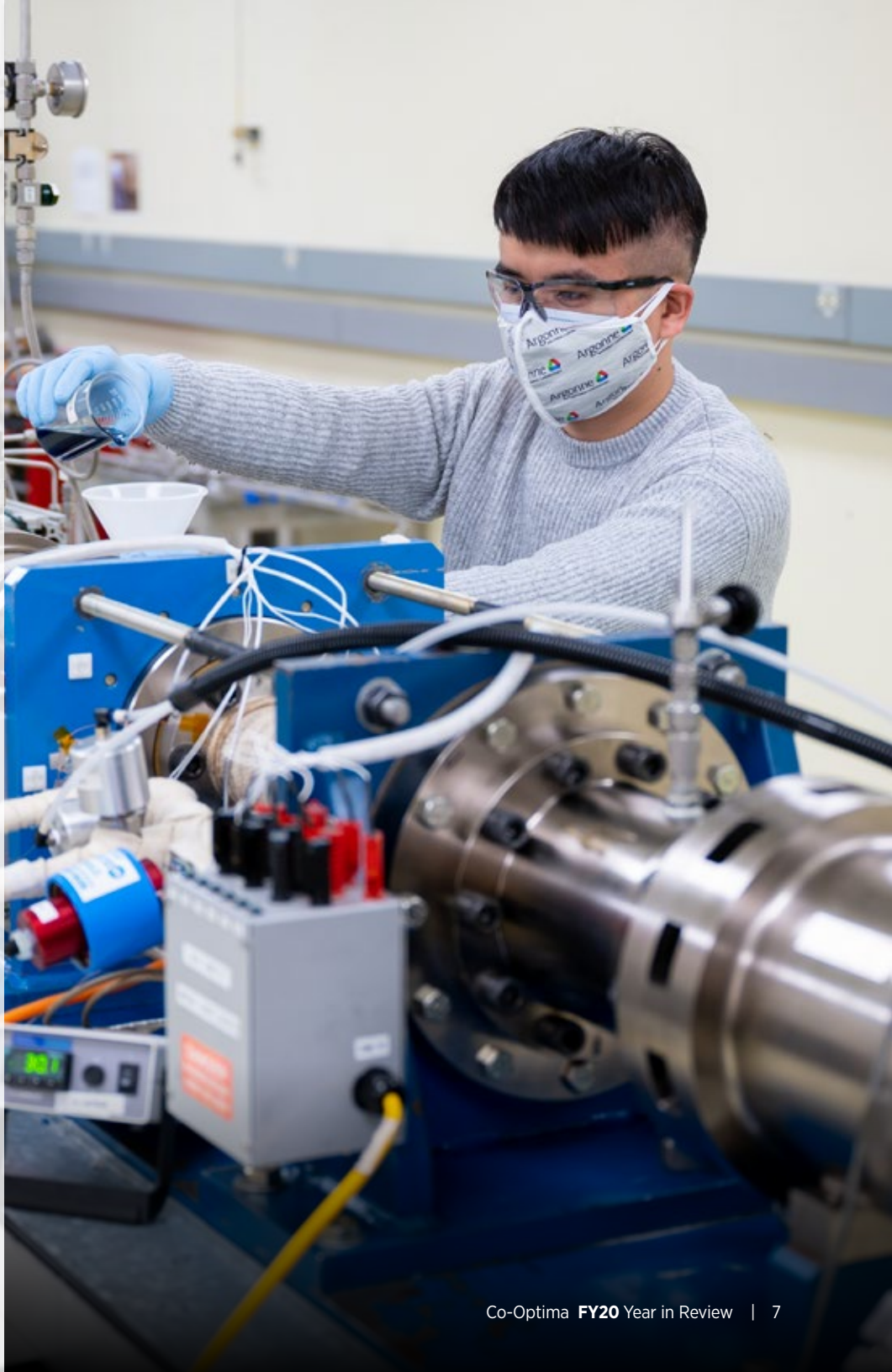


Photo: ANL

STAKEHOLDERS HELP NAVIGATE CO-OPTIMA PRIORITIES

From the start, the Co-Optima team has engaged external stakeholders from across the fuel and vehicle industries, as well as from government agencies and research institutions. Regular input on stakeholder priorities and needs has made it possible to better gauge potential research directions and market viability of innovations of the Co-Optima initiative. In past years, stakeholders and research team members have come together at "listening day" events, trade association conferences, one-on-one stakeholder meetings, DOE review meetings, and meetings of Co-Optima's external advisory board.

Even with FY20 conferences cancelled or moved to a virtual format due to the pandemic, Co-Optima researchers continued contributing to important science and engineering forums sponsored by organizations such as the Advanced Bioeconomy Leadership Conference (ABLC), SAE International, Combustion Institute, American Institute of Chemical Engineers, American Chemical Society, and Algae Biomass Organization (ABO). Co-Optima researchers have also continued to provide monthly stakeholder and quarterly advisory board updates. These exchanges of knowledge and ideas—virtual or in person—are essential to ensuring that Co-Optima research and development (R&D) targets those scientific and engineering challenges viewed as most important and valuable by the larger research and stakeholder communities.

To increase near-term market impact, in FY20 DOE provided a new opportunity for stakeholders to work directly with Co-Optima National Laboratories on R&D most relevant to industry aims. DOE selected seven projects via a competitive Directed Funding Opportunity (DFO) to establish cooperative research and development agreements led by industry partners while leveraging the unique experimental and computational capabilities of the National Laboratories. The industry partners are contributing a market-facing perspective, specific complementary expertise, and cost sharing to address specific research barriers at the fuel-engine interface.

The selected Co-Optima DFO projects are:

- ExxonMobil Research and Engineering Company and Argonne National Laboratory (ANL) are developing a life cycle analysis modeling framework to estimate the greenhouse gas emissions produced by refinery coprocessing of renewable fuels.
- General Motors, Oak Ridge National Laboratory, and the National Renewable Energy Laboratory (NREL) are determining fuel property effects on abnormal combustion for biofuel-petroleum fuel blends.
- LanzaTech and Pacific Northwest National Laboratory (PNNL) are demonstrating the production of a gasoline-range fuel with advanced fuel properties.
- CFR Engines and ANL are developing a fuel reactivity metric and test method for advanced compression ignition combustion engines.
- Shell and NREL are applying metabolic engineering and process optimization to the biological production of the high-performance blendstock isopropanol.
- Sylvatex and ANL are evaluating the injector performance of Sylvatex's alternative diesel fuel and optimizing its formulation.
- Visolis and PNNL are converting Visolis' bioderived intermediate into a high-energy-density blendstock for use in gasoline engines.

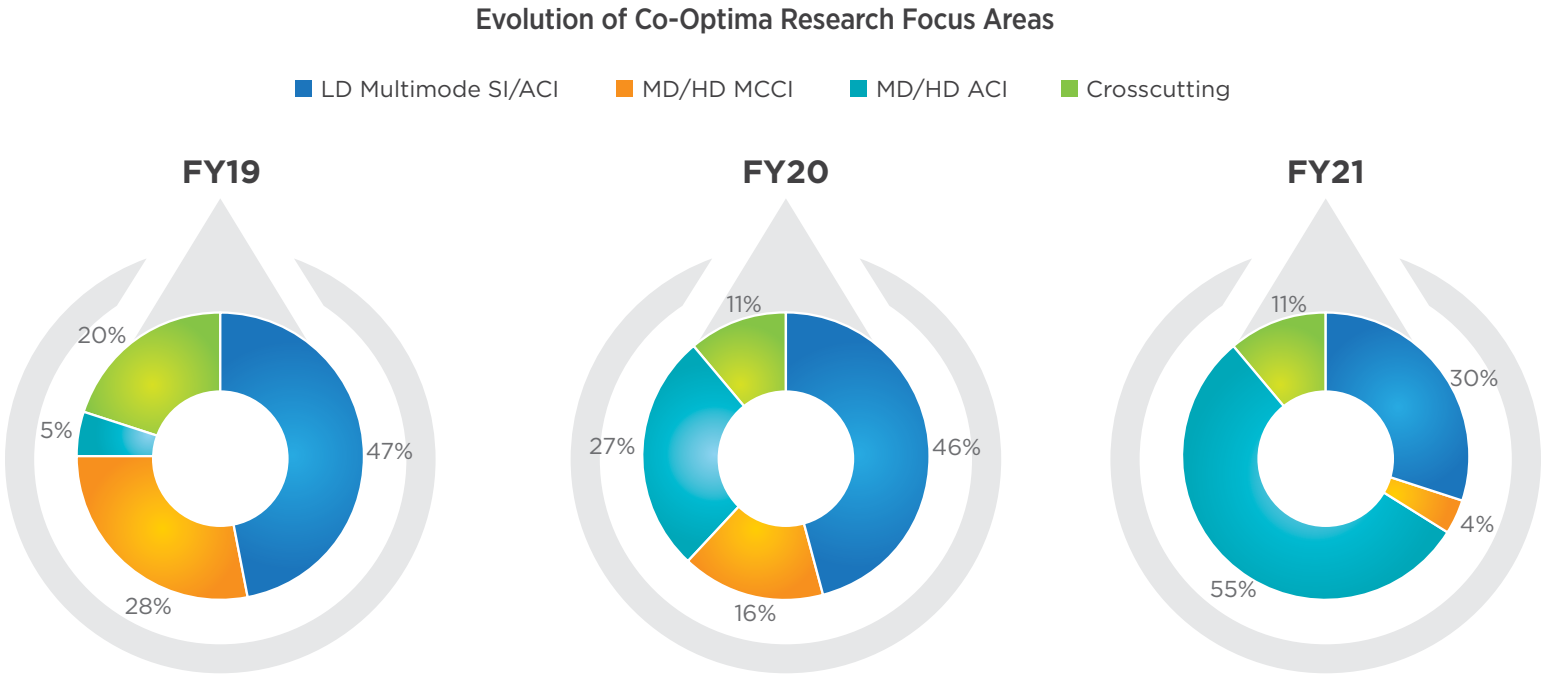
Results of research funded in this round of DFO awards will be spotlighted in next year's *Year in Review* report.

TECHNICAL RESEARCH ACCOMPLISHMENTS AND IMPACT

FY20 Co-Optima research focused on multimode combustion strategies for LD vehicles and MCCI and ACI strategies for MD and HD vehicles. By concentrating on the relationship between fuel molecular structure and properties, as well as how fuel properties impact engine operation, researchers were able to devise strategies for further improving efficiency, reducing emissions, and using blendstocks derived from renewable domestic feedstocks.

Significant progress was made in understanding blending effects on autoignition chemistry (needed to help alleviate harmful engine knock) and the connection between molecular structure and soot formation (essential to reducing particulate emissions). Researchers used this approach to define critical properties for three LD multimode combustion approaches. An improved understanding on both fronts was used to identify multimode and MCCI blendstocks that demonstrate the potential to meet economic and environmental targets. Engine combustion research on MCCI blendstocks was initiated, and structure-property relationships for phi-sensitivity—a new fuel property that reflects how a fuel's autoignition reactivity changes as a function of phi (the fuel-to-air equivalence ratio) and is critical for some ACI strategies—were investigated in detail.

Highlights of the most significant FY20 Co-Optima accomplishments can be found in the following sections.



Analysis

Bookending Research with Upfront Estimates and Conclusive Assessments

Which new biobased fuels and production pathways warrant a closer look? What benefits can widespread adoption of co-optimized fuel and engine technologies provide? Analysis guides Co-Optima research at every step—from discovering viable high-performance fuel candidates to measuring their efficiency and emissions benefits when paired with a variety of combustion strategies.

Upfront analysis steers early Co-Optima blendstock evaluation with estimates of fuel costs and environmental performance, enabling researchers to focus on the most promising options. Later, teams feed experimental data back into the analyses to refine estimates and benchmark progress. Finally, analysis puts new technologies' performance in context with assessments of their potential benefits and trade-offs at market scale.

Techno-economic analysis (TEA) is used to evaluate the economic performance of a given process or system. Co-Optima researchers use TEA to understand the potential of a proposed process compared to established standards and identify areas that require further R&D.

While TEAs are often only performed once key data from experiments are in hand, Co-Optima analysts work with researchers to conduct screening analyses early in the research process, often assuming close-to-ideal values prior to making any experimental measurements. As more experimental information becomes available, analysts generate more-detailed models of cost and environmental performance to identify the most promising blendstocks.

In FY20, Co-Optima analysts and researchers completed parallel assessments of multimode and MCCI blendstocks for LD, MD, and HD engines. Analysts compiled data on 19 factors related to technology readiness, economic viability, and environmental impacts to identify the most promising bioblendstocks from an array of candidates.

Detailed process modeling and integrated TEA and life cycle analysis were then conducted to identify an even smaller pool of nine multimode and seven MCCI blendstock candidates with the greatest potential to help Co-Optima meet targets of reducing GHG emissions by at least 60% while delivering strong efficiency and performance and minimizing other environmental impacts.

Meanwhile, Co-Optima researchers identified properties of candidate fuels that could also offer the greatest profitability to the U.S. refining industry, with the feasibility to be produced at commercial scale while delivering prices at the pump of less than $5.50 per gasoline gallon equivalent. In addition, the experimental fuel properties research combined with the analyses confirmed that co-optimized fuels and engines could increase efficiency and reduce GHG emissions while playing an important role in improving U.S. energy security and the competitiveness of the U.S. automotive sector.

More details on Co-Optima analysis accomplishments can be found in the technical highlights throughout the following sections.

Photos: LBNL, ANL, SNL (left to right)

New Tools

Evaluation of Fuel Blends in Days, Rather than Months

Simulating fuel blend performance is much faster than evaluating blends experimentally in internal combustion engines and can reduce the need for costly prototyping and testing. However, this requires predictive tools that can accurately capture fuel-engine interactions and powerful computing resources to speed up computations.

The Co-Optima team has developed multiple computational tools and models to improve the efficacy of predictions and reduce computation costs. These include high-fidelity computational fluid dynamics (CFD) simulations that provide new insights on fuel-engine interactions. The team has also developed lower-fidelity models that can still deliver the accuracy needed for fuel-engine co-optimization by leveraging acceleration techniques based on high-performance computing (HPC) and machine learning.

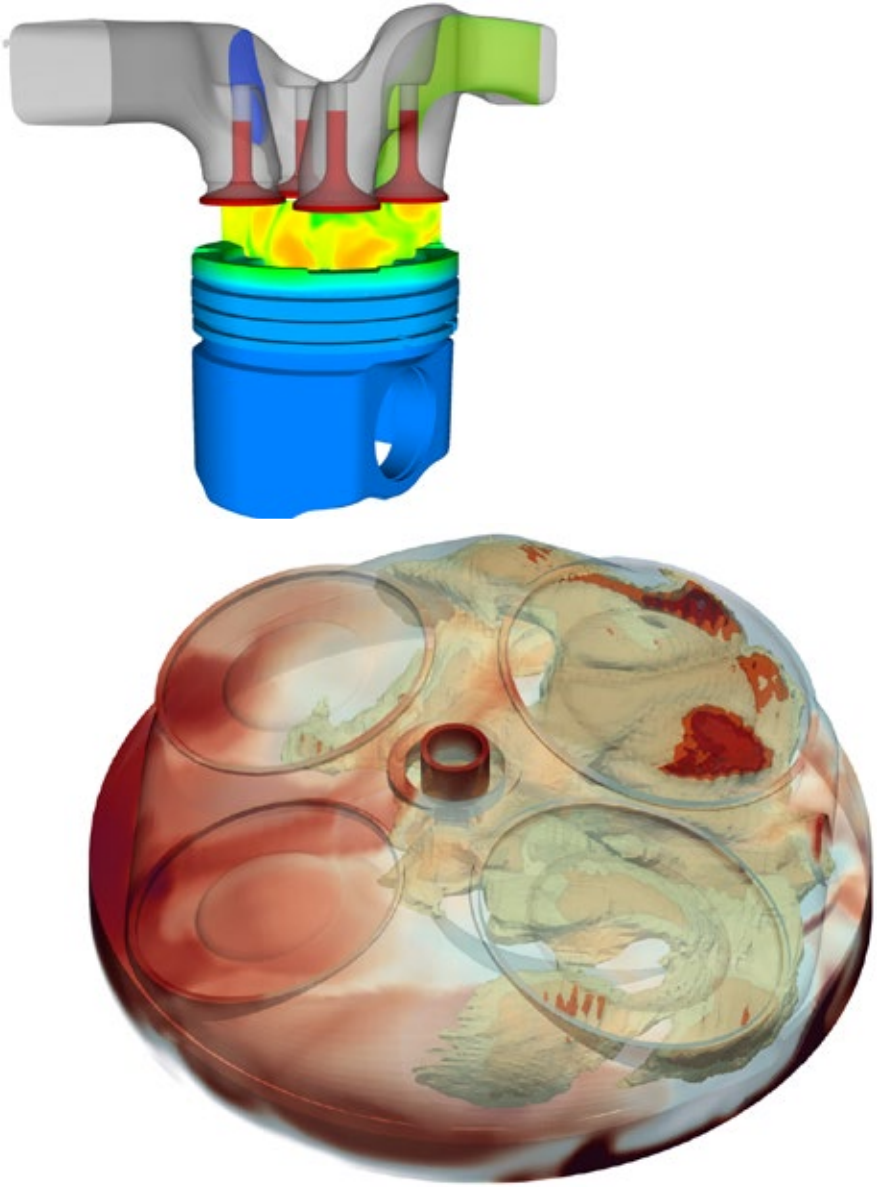
These innovative new tools and models include:

In-Nozzle Flow and Spray Modeling

- Multiphase flow modeling for diesel and gasoline fuel injection nozzle hardware
- Enables the accurate evaluation of evaporation from liquid-fuel films, whose residual mass is linked to soot formation
- Used in studies of fuel effects on phenomena like flash boiling, multicomponent film vaporization, and ducted fuel injection.

Models for Different Combustion Regimes

- Robust model for different combustion regimes such as boosted SI, spark-assisted compression ignition (SACI), and ACI
- Evaluates the effect of fuels' physical and chemical properties
- Used to capture such properties as pre-spark heat release and pre-chamber-based combustion flows.



Figures by ANL

Computational Solvers for Different Combustion Regimes

- Robust model for different combustion regimes such as boosted SI, SACI, and ACI
- Laminar solver that allows flame speeds to be computed several orders of magnitude faster than with standard tools
- Used to capture the effect of full chemistry mechanism on flame propagation and end-gas autoignition.

Lower-Fidelity Models to Predict Engine Performance

- Chemkin-Pro-based engine model for SACI multimode operation, which runs much faster than a CFD calculation
- Lower-order simulations accelerated by 40 times using Zero-order Reaction Kinetics (Zero-RK) software to allow evaluation of components in 50,000 fuel blends.

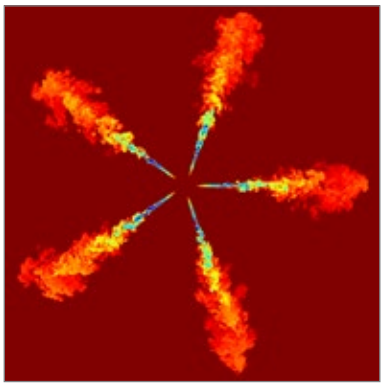
Gaussian Process (GP) Optimization Algorithm

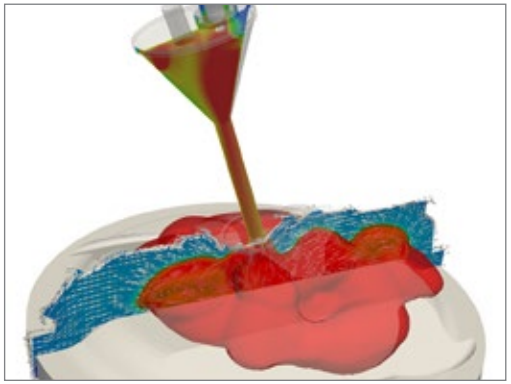
- Algorithm that identifies subsets of blend candidates for engine simulations
- Zero-RK model results integrated into the GP algorithm to predict which blends might provide optimal engine performance
- Neural network framework to predict octane (and other properties) using ignition properties from the detailed Co-Optima kinetic mechanism (~3,000 species).

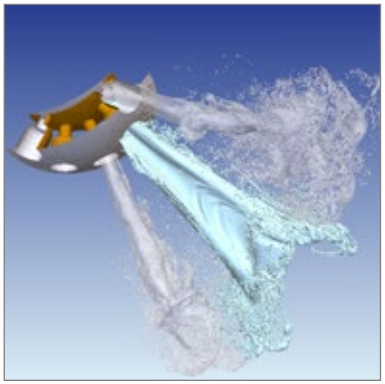
These new tools have been rigorously validated with optical and metal engine platforms for many fuels at several National Laboratories. Leveraging HPC resources, new approaches for two-phase flows, and combustion modeling have been made available through user-defined functions, allowing the engine industry to plug routinely used commercial codes into the models. The fast solvers, lower-order models, and GP algorithms have made it possible to evaluate an unprecedented number of fuel blends in days rather than months.

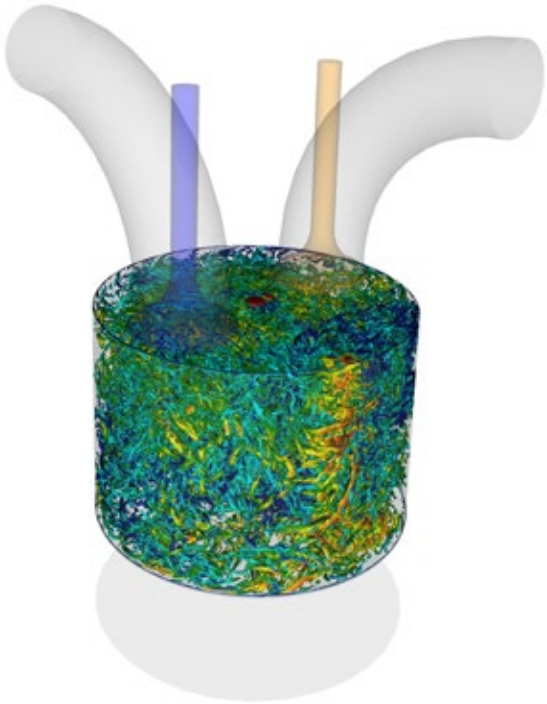
While Co-Optima's initial tool development supported LD boosted SI and multimode activities, Co-Optima research has shifted to more MD and HD compression ignition engine simulations. Future modeling and simulation work will leverage developments within DOE's Partnership for Advanced Combustion Engines (PACE) and Exascale Computing Project (ECP), along with the latest advancements in artificial intelligence and machine learning.

Information on other tools and data available on the Co-Optima website can be found at the end of this report.









Figures by ANL

Light-Duty Fuel and Engine Research

Multimode Breakthroughs: 10 New Viable Biobased Blendstocks for Light-Duty Vehicles

Engines that use boosted spark ignition (SI) under high-load conditions and advanced compression-ignition (ACI)/lean-SI modes under part-load conditions are known as multimode engines. SI engines are most efficient at high engine loads but lose efficiency in the low- and intermediate-load conditions that make up most real-world driving. ACI and lean-SI combustion modes and engine technologies can boost efficiency and cut emissions under these low- and intermediate-load conditions while maintaining power density and efficiency gains through turbocharging, direct injection, engine downsizing, and downspeeding. Many different light-duty (LD), medium-duty, and heavy-duty vehicles may benefit from a range of multimode strategies.

In Fiscal Year 2020 (FY20), Co-Optima researchers continued to build on a foundation of research dedicated to boosted SI combustion strategies, establishing critical fuel properties and identifying high-performance blendstocks that can enable three multimode approaches for LD vehicles: ACI, spark-assisted compression ignition (SACI), and lean-stratified SI. Analysis reveals each of these 10 blendstocks can potentially be produced at a competitive price and reduce greenhouse gas (GHG) emissions by at least 60% compared to petroleum-based fuel.

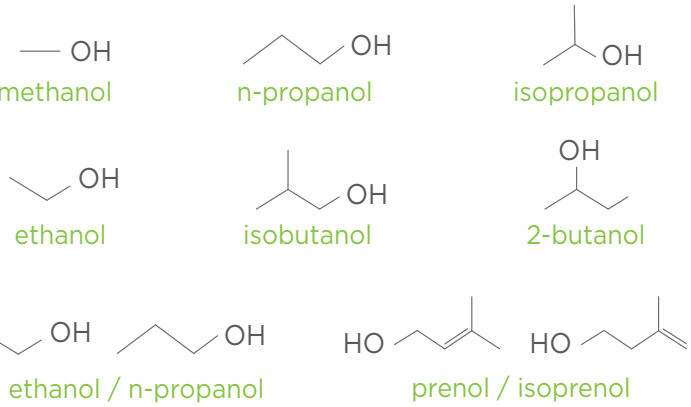
Co-Optima research on multimode combustion examined chemical kinetics; relationships between molecular structure, fuel properties, and performance; combustion strategies; blendstock properties; and economic and life cycle impacts. The three key multimode combustion strategies have similar—though not identical—requirements to maximize performance, efficiency, and environmental benefits. Bioblendstocks were identified based on four criteria: offering fuel properties compatible with anticipated combustion modes, reducing life cycle carbon emissions, showing potential for high market penetration, and demonstrating synergistic blending for research octane number.

All of these criteria were met by methanol, lignocellulosic ethanol, n-propanol, 2-propanol (also known as isopropanol), isobutanol, 2-butanol, a prenol/isoprenol mixture (50/50 by weight), an ethanol/propanol mixture (90/10 by weight), di-isobutylene, and a methylfuran/dimethylfuran mixture (40/60 by weight). Of these, lignocellulosic ethanol is already a market fuel and isopropanol, n-propanol, isobutanol, di-isobutylene, and the ethanol/n-propanol mixture have the fewest barriers to adoption.

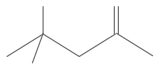
Select Co-Optima accomplishments related to multimode combustion co-optimized with high-performance fuels in LD vehicles can be found in the following section.

Blendstocks with Highest Merit Function Scores for LD Multimode Engines

Alcohols

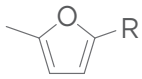


Olefins



di-isobutylene

Furans



R=-H, -CH

furan mixture

Photo: PNNL

TAILORED OXYGENATES FROM DIRECT CATALYTIC CONVERSION SHOW PROPERTIES FIT LD FUELS

Achievement: Researchers tailored the composition of mixed oxygenate biofuels through surrogate property-informed process design to meet target fuel properties.

Potential Impact: The biofuel product of the DC3 process has higher energy density, lower freezing point, and decreased vapor pressure relative to E10, highlighting its potential for use in light-duty boosted SI and multimode engines.

The direct catalytic conversion of cellulosics (DC3) process upgrades lignin-removed woody biomass into light oxygenates with high yields. However, to date, examination of the product fuel properties has been limited. Co-Optima researchers created several 20-component fuel surrogates based on detailed chemical analysis of DC3 products to determine their fuel properties and compatibility. In addition, delignified biomass was solubilized in supercritical methanol and catalytically upgraded to produce mixed C2–C6 oxygenates (molecules containing two to six carbon atoms). Surrogate DC3 fuels were used to inform catalyst and process condition selection to increase the carbon yield of larger alcohols. Findings were then applied to DC3 process-delignified poplar. Both the surrogate and woody biomass-derived DC3 10% biofuel blend in gasoline were shown to have higher energy density, lower freezing point, and decreased vapor pressure relative to E10 (10 vol % ethanol). Additional research is needed to clarify the potential environmental and economic impacts of DC3 production.

Fuel Property	RBOB	E10	Surrogate 10% Blend	Biofuel 10% Blend
LHV (MJ/kg)	42.83	38.8	44.2	41.7
Density (g/mL)	0.744	0.73	0.764	0.756
RON	87.5	92.7	88.6	87.5
Sensitivity	6.9	9.2	6.3	5.2
RVP (psi)	5.28	6.40	6.12	-
HOV (kJ/kg)	359	418	384	363
Cloud Pt. (°C)	< -70 (est.)	< -40	< -75	< -75
T90 (°C)	171	168	173	198

Residual cellulosics are upgraded to mixed light oxygenates using the DC3 process. Fuel properties were measured for a model DC3 blendstock surrogate and a woody biomass-derived DC3 blendstock blended at 10% in reformulated blendstock for oxygenate blending (RBOB). Improvements of the DC3 surrogate blend and biofuel blend relative to E10 are shown in green. HOV = heat of vaporization, LHV = lower heating value, RON = research octane number, RVP = Reid vapor pressure, T90 = distillation temperature at which 90% of the fuel (by volume) evaporates. Figure by Nabila Huq, Hannah Nguyen, and Derek Vardon, NREL

HOMO-ISOPRENOID ALCOHOL BLENDSTOCKS PRODUCED VIA SYNTHETIC BIOLOGY HAVE PROMISING FUEL PROPERTIES

Achievement: Synthetic biology was used to produce six- and seven-carbon homo-isoprenoid alcohol blendstocks.

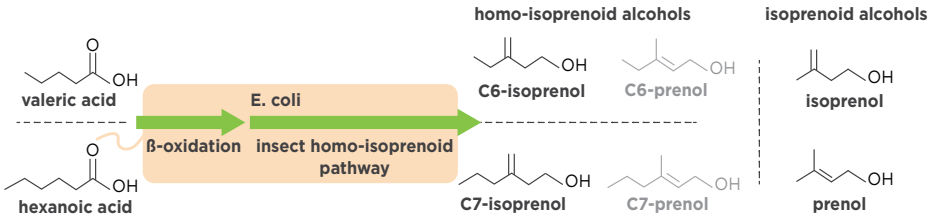
Potential Impact: When paired with boosted SI and multimode engines, the novel blendstocks promise higher RON, lower water solubility, and greater energy density than those found with more established biofuel candidates.

Because of their high octane sensitivity and synergistic blending for research octane number (RON), the isoprenoid alcohols prenol and isoprenol are promising blendstocks for boosted SI and multimode ignition strategies. Traditional biochemical pathways yield alcohols with five-carbon chain lengths. This research explored the feasibility of producing homo-isoprenoid alcohols with six- and seven-carbon atoms.

Fuel property modeling indicates that these molecules with longer carbon chains are likely to deliver better RON, water solubility, and energy density than their five-carbon analogs. At the same time, developing these types of molecules using currently available chemical synthesis techniques has been hampered by cost, complexity, and safety concerns. Recent advances in genetic engineering, in which microbes are engineered to become "cell factories" for production of useful molecules, make biosynthetic production a promising alternative method.

To extend the carbon chain of isoprenoid alcohols, the team expressed the homo-isoprenoid biosynthetic pathway genes from *Bombyx mori*, the domestic silkworm, in *Escherichia coli*, a commonly engineered bacterial strain. Coupling the homo-isoprenoid pathway with the β-oxidation pathway, by which fatty acid molecules are broken down in living organisms, researchers redirected this pathway to use valeric acid, a platform molecule produced from woody plants' lignocellulose, to produce six-carbon isoprenol.

They then adapted the pathway to use hexanoic acid, a fatty acid common in animal fats and oils, to produce seven-carbon isoprenol. This work demonstrates the potential for synthetic biology to produce biofuels with superior properties when compared to the current canonical set of candidate molecules available via biosynthetic pathways.



Compound	Predicted RON	Predicted LHV (MJ/kg / MJ/L)	Predicted Water Solubility (g/L)
isoprenol	97.2*	37.3 / 31.45	36
prenol	93.5*	34.038* / 28.66*	46
C6-isoprenol	97.9	38.5 / 32.1	15
C6-prenol	101.2	38.5 / 32.5	19
C7-isoprenol	96.2	39.4 / 32.9	5.8
C7-prenol	88.4	39.4 / 33.3	7.3

Microbial production pathway of homo-isoprenoid alcohols and their predicted fuel properties. The production of six-carbon (C6) and seven-carbon (C7) isoprenols has been confirmed, while molecules in grey are possible via adaptation of the newly developed pathway. These homo-isoprenoid alcohols are analogs to the five-carbon isoprenoid alcohols, currently established as biofuel candidates. Asterisks (*) denote property metrics that reflect experimental measurements. Figure by Bo Pang and Ethan Oksen, LBNL

LOW-AROMATIC BASE FUELS ACCENTUATE PRENOL'S SYNERGISTIC OCTANE BLENDING

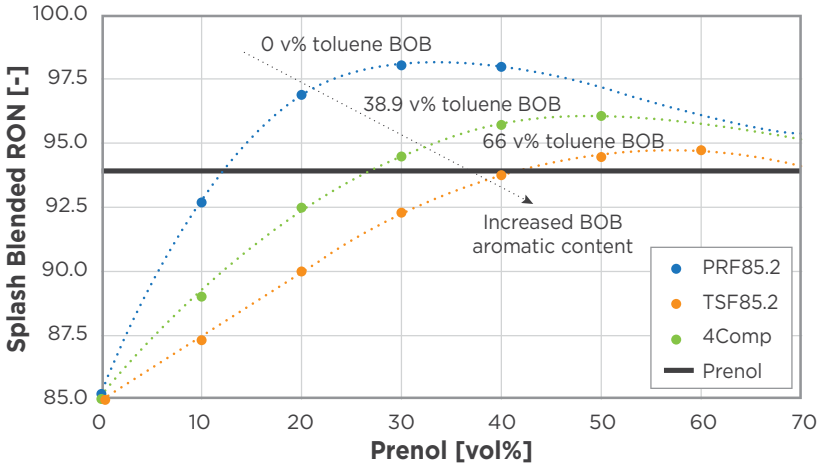
Achievement: Experiments showed that prenol's synergistic RON effect was largest when prenol was blended into a zero-aromatic BOB, but the effect declined as the BOB toluene content increased.

Potential Impact: Prenol must be blended with low-aromatic BOBs to obtain maximum synergistic blending and enhance the performance of multimode and SI engines at potentially reduced cost.

Co-Optima researchers previously identified prenol, a renewable olefinic alcohol, as a "hyperboosting" blendstock. This means that prenol exhibits highly synergistic octane blending—the RON of prenol-gasoline blends can be higher than the individual RONs of the neat prenol and the base gasoline. Higher RON can enhance the performance of multimode and SI engines.

Researchers investigated this phenomenon further by experimenting with prenol blended into three gasoline blendstock for oxygenate blending (BOB) surrogates with the same RON (85.2) and three levels of aromatic (toluene) content: 0% (by volume) toluene in a primary reference fuel (PRF 85.2), 38.9% in a four-component BOB surrogate (4Comp), and 66% in an ASTM toluene standardization fuel (TSF 85.2). The researchers found that PRF 85.2 accentuated prenol's synergistic blending effect the most. Aromatics in the BOB suppressed the RON gain and shifted the blend with the maximum RON value from 30% prenol (in PRF 85.2) to 60% prenol (in TSF 85.2).

By investigating the Cooperative Fuel Research (CFR) engine operating conditions and combustion and knocking characteristics during the RON tests, the researchers found that prenol's synergistic octane blending was not simply a function of the unique characteristics of the ASTM RON test method. When modified RON ratings were generated under stoichiometric conditions and based on a cylinder pressure transducer knock intensity metric, prenol's synergistic blending effect was still observed. This means it is likely that prenol's knock resistance in the CFR engine will translate to multimode and SI engines.



RON vs. percentage of prenol blended in BOBs with different aromatic (toluene) content, compared with the RON of neat prenol, showing the diminishing synergistic blending effect as BOB aromatic content increases. Figure by Christopher Kolodziej, ANL

SEVEN BIOBLENDSTOCKS DEMONSTRATE OCTANE HYPERBOOSTING WITH POTENTIAL FOR GREATER LD ENGINE EFFICIENCY

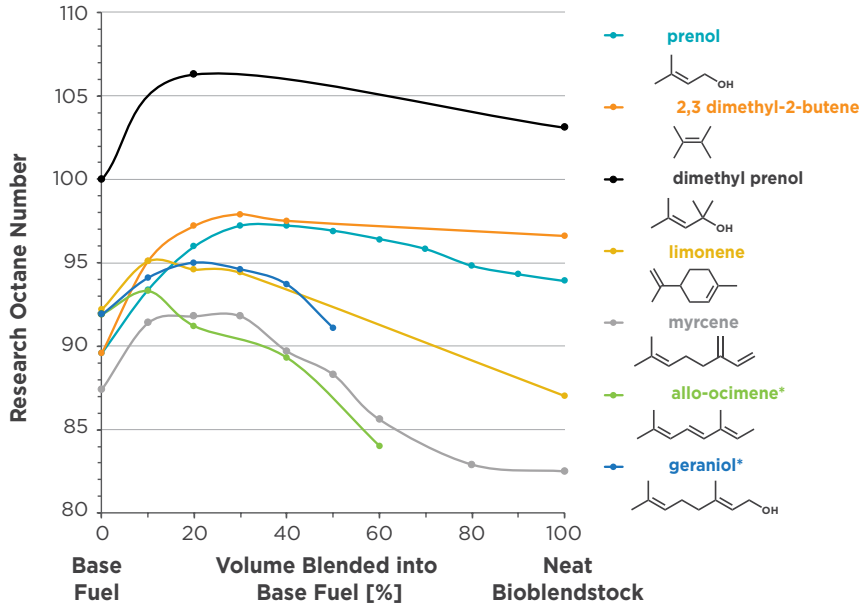
Achievement: Researchers discovered seven new bioblendstocks and the corresponding molecular characteristics that lead to RON hyperboosting—a phenomenon previously only observed with prenol.

Potential Impact: Hyperboosting blendstocks may provide a less expensive path to increasing octane.

Fuels with a high RON are essential for efficient LD SI engines. Although a fuel blend's maximum RON is typically limited to the sum of the weighted average of the RONs of its individual pure components, when a hyperboosting blendstock is blended with a gasoline BOB, the RON of the blend can be higher than both the RON of the blendstock and the RON of the BOB.

While this effect had previously only been observed in prenol blends, Co-Optima researchers systematically searched for it in a bounded set of closely related structures and conducted engine tests to determine the behavior of the candidate blendstocks. Of the structures considered, seven new compounds—three branched unsaturated alcohols and four branched alkenes—exhibited RON hyperboosting to varying degrees. Among these, dimethyl prenol had the highest blending RON, corresponding to a 10 vol % blending RON of 147, which is higher than that of prenol and seven of the molecules identified by earlier Co-Optima research as the top-10 candidates for use in boosted SI engines.

The team is currently using results of this research and computational modeling to identify and test potential kinetic mechanisms for the hyperboosting effect. This mechanism could have important implications for combustion science, the production of fuels from biomass, and future vehicle efficiency.



Experimental RON results demonstrating octane hyperboosting by seven bioblendstock candidates when blended into a base fuel. The neat RON for compounds with an asterisk could not be measured, but these compounds exhibited the critical inflection point in the RON curve indicative of hyperboosting. Figure by Eric Monroe, SNL

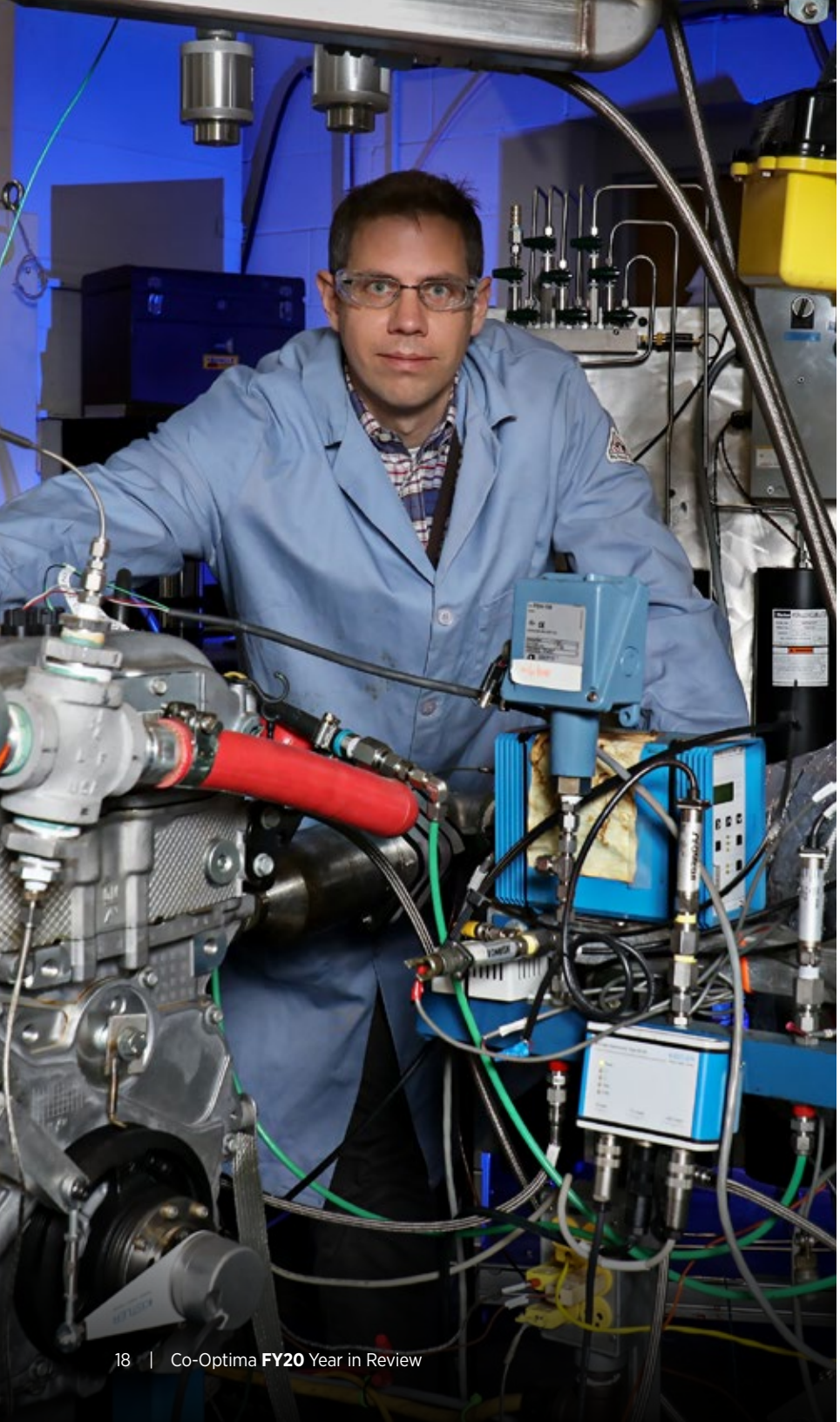


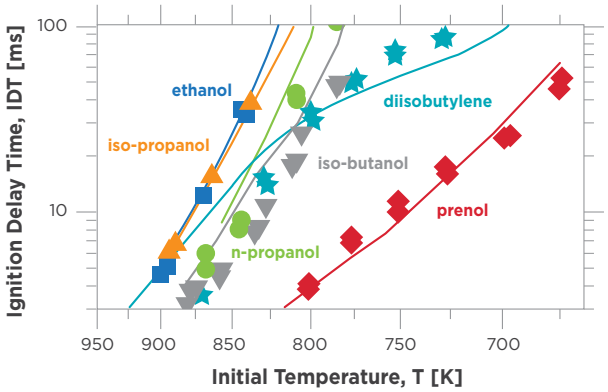
Photo: ORNL

IMPROVED CHEMICAL KINETIC MODELING MORE ACCURATELY REFLECTS BEHAVIOR OF CO-OPTIMA BLENDSTOCKS IN GASOLINE BASE FUELS

Achievement: Co-Optima's chemical kinetic modeling capabilities were improved to more accurately represent the nonlinear blending behavior of Co-Optima blendstocks in petroleum refinery gasolines.

Potential Impact: The improved kinetic models can more accurately evaluate combustion of promising blendstocks in gasoline base fuels under conditions relevant to multimode and advanced compression-ignition engine strategies, leading to higher efficiency, fuel-optimized engine designs.

Chemical kinetic models are used in engine simulations to assess the effects of fuels on combustion processes. Researchers improved Co-Optima's kinetic modeling capabilities to more accurately represent the chemistry of blendstocks and the base gasolines into which they are blended. New or improved kinetic models were added for ethanol, n-propanol, isopropanol, isobutanol, prenol, and diisobutylene—all of which have been identified by Co-Optima researchers as among the 21 most promising blendstocks for multimode engines. The kinetic models were validated against rapid-compression machine (RCM) measurements of ignition delay time. Additional experimental data from Co-Optima researchers and the literature, including flow reactor and jet-stirred reactor data, were also used to improve the modeling. The models can be used to simulate engine pressure-temperature trajectories to investigate the impact of blendstocks on combustion phasing, heat release rates, engine knock, and misfire. The researchers blended isopropanol and isobutanol in FACE-F (a research-grade gasoline base fuel) and studied the blends in an RCM, validating the models' ability to capture the fuel's decreasing autoignition reactivity as the amount of blendstock increases. The models also can be used to design surrogate mixtures for gasoline fuels by matching properties such as RON and octane sensitivity.



Simulations (lines) and RCM measurements (symbols) of ignition delay time vs. initial temperature for stoichiometric mixtures of six Co-Optima blendstocks at pressures of 30–40 bar. Initial temperature refers to the thermodynamic state after compression in an RCM when time is defined as zero. RCM measurements for ethanol, n-propanol, isopropanol, and isobutanol are from Co-Optima researchers, while diisobutylene and prenol measurements are from National University of Ireland Galway (NUIG). When blended with gasoline base fuels, these blendstocks increase the RON of the resulting fuel. Figure by Scott W. Wagnon, LLNL, and Nitin Lokachari, NUIG

EXPERIMENTS AND MODELING CLARIFY THE MECHANISMS OF SYNERGISTIC BLENDING, INFORM DEVELOPMENT OF HIGH-VALUE BIOBLENDSTOCKS

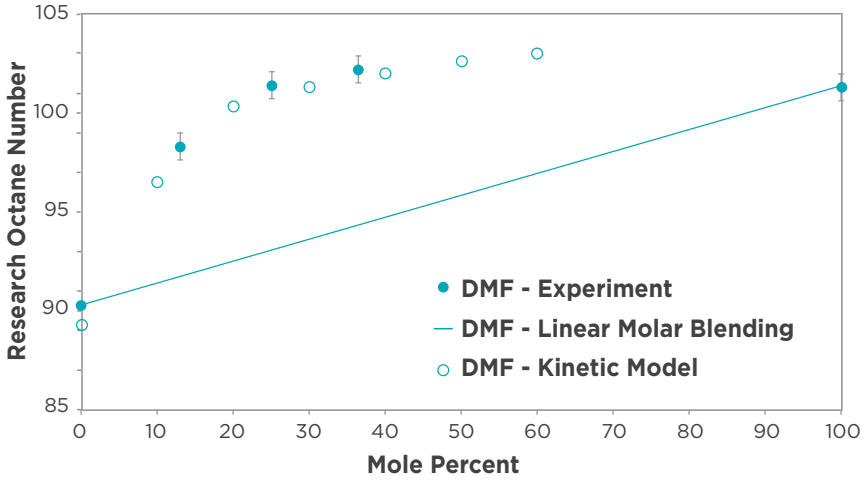
Achievement: Combining kinetic simulations and flow-reactor experiments clarified the chemical mechanisms responsible for synergistic blending.

Potential Impact: Understanding the mechanisms of synergistic blending can ensure future fuels take full advantage of highly synergistic blendstocks and enable development of combustion strategies to exploit those blendstocks' unique properties.

When some bioblendstocks are blended with petroleum gasoline, the RON can be significantly higher than predicted by a linear blending model—a synergistic effect that adds economic value to the bioblendstock. The mechanism of this effect, however, is not well understood. Co-Optima researchers investigated it by measuring RON for various blendstocks blended with a surrogate gasoline and using kinetic simulations to study the autoignition chemistry.

Dimethylfuran (DMF) exhibited one of the highest levels of synergy, translating into one of the highest levels of RON. Kinetic simulations showed that the gasoline surrogate exhibits two-stage autoignition: low-temperature heat release (LTHR) followed by the main autoignition. Blending with 20% DMF eliminated the first-stage ignition. Interrogating the kinetic model to determine the most important reactions showed that the gasoline surrogate reacts with oxygen and hydroxyl radical to initiate low-temperature chain branching below 750 K when DMF is not present. Upon blending with DMF, it preferentially reacts with oxygen and hydroxyl radical in chain-terminating reactions, leading to a delay in autoignition and a boost in RON. At temperatures of 750–900 K, DMF reacts primarily with hydroxyl radicals in chain-terminating reactions.

The combination of reactions with oxygen and hydroxyl radicals—preventing them from reacting with other fuel components—makes DMF such an effective synergistic blending component. Kinetic simulations were used to generate a list of the top species produced from DMF blends, shedding light on the chemical mechanisms responsible for radical scavenging. Observation of these species in flow-reactor experiments validated predictions from the simulations. This knowledge of synergistic blending and the important reactions that cause RON synergy can facilitate development of valuable bioblendstocks.



RON vs. molar percentage of DMF blended with a surrogate gasoline, measured data and predictions via kinetic simulations. Comparison to the linear molar blending line shows the extent of synergistic blending, which is well captured by the kinetic model. Figure by Robert L. McCormick, NREL

OPTIMIZATION ALGORITHM COUPLED WITH ENGINE SIMULATOR FINDS BETTER FUEL BLENDS FASTER

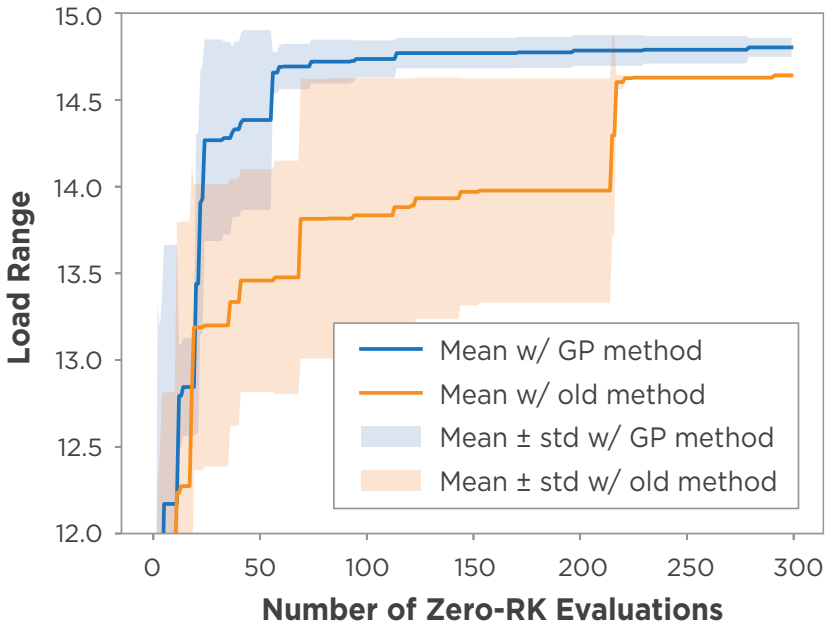
Achievement: Researchers developed an optimization algorithm that accelerates and enhances the identification of potentially optimal fuel blends for use in advanced engines and demonstrated this approach for the case of SACI combustion.

Potential Impact: The algorithm enables rapid identification of fuels suitable for laboratory performance testing, which significantly decreases resource requirements during the search for new fuels.

Simulating the performance of fuel blends in advanced engines is much faster than testing in real engines. However, even when simulations are employed, the immense number of possible blends constrains the speed and scope of optimal fuel blend searches. Co-Optima researchers helped accelerate these searches by developing a Gaussian process (GP) optimization algorithm that quickly identifies optimal blend candidates from simulations.

The researchers demonstrated the algorithm using Lawrence Livermore National Laboratory's Zero-order Reaction Kinetics (Zero-RK) implementation of Sandia National Laboratories' model of SACI. The GP algorithm helped these models optimize fuel blends based on nine chemical species from among five fuel groups: paraffins, isoparaffins, olefins, naphthenes, and aromatics. The target was to maximize the load range (the difference between the highest and lowest power for stable SACI operation). Increased load range indicates an increase in the time that an engine operates in the more-efficient mode during a drive cycle.

Across five independent trials, the load range values were very similar (within 2% of one another) for each optimized blend. However, the compositions of the optimized blends differed across trials, likely owing to the existence of multiple local minima or relatively flat regions of the optimization landscape; this means that multiple blend options may provide the same performance. The GP algorithm outperformed the previously used genetic algorithm in terms of convergence speed and solution quality. In addition, the GP algorithm can be easily generalized for application to a broad range of simulation models.



Load range vs. number of Zero-RK SACI engine simulations run during a search for optimal fuel blends, assisted by the GP algorithm ("GP method") or by a genetic algorithm ("old method"); higher values equate to better fuel blends. The lines are the mean values across five optimization trials, and shaded fields represent ±1 standard deviation around each mean. Figure by Juliane Mueller (LBNL) and Matthew McNenly (LLNL)

DETAILED UNDERSTANDING OF MOLECULAR INTERACTIONS EXPLAINS VAPOR PRESSURE CHANGES

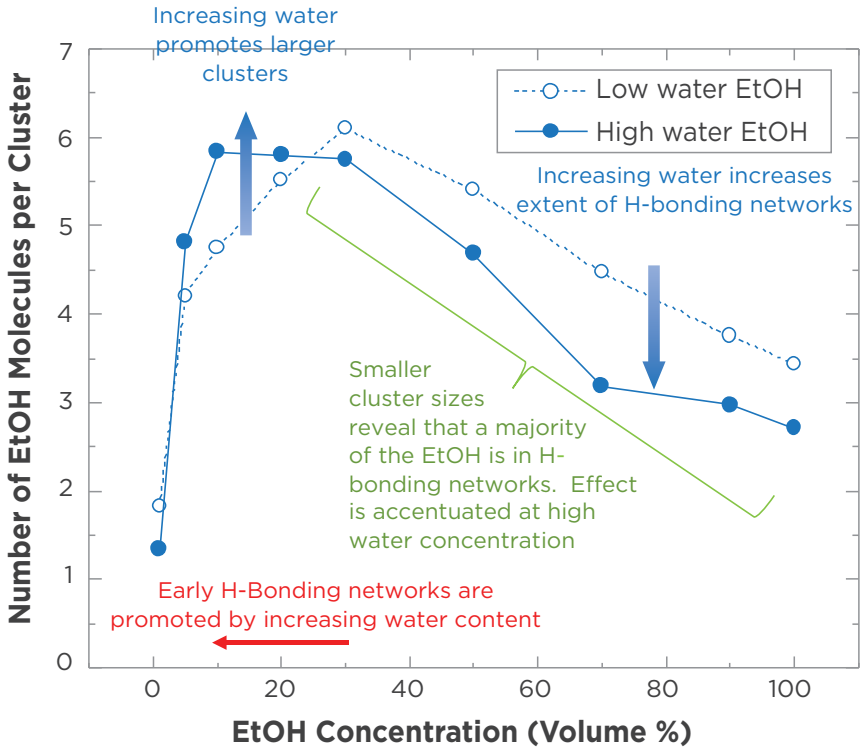
Achievement: Small differences in water content in a surrogate fuel with 10% ethanol by volume were shown to predictably change the size and size distribution of alcohol clusters and increase fuel vapor pressure by about 6%.

Potential Impact: Improved understanding of the molecular origins of this thermodynamically nonideal behavior in fuels may facilitate fuel property or fuel blending predictions that better accommodate molecular-scale interactions.

The extent of hydrogen bonding among fuel molecules, fuel additives, or impurities governs molecular-scale organization that occurs within a fuel—and affects fuel behavior during storage, transport, and use. For example, fuel vapor pressure reflects the aggregate intermolecular forces within the fuel. Previous Co-Optima research showed correlation between increased alcohol cluster size and increasing fuel vapor pressure.

In FY20, the researchers showed that changes of only a few thousand parts per million (ppm) in water content altered the balance between clustering and hydrogen-bonding networks within an alcohol-containing surrogate fuel, affecting fuel vapor pressure. The researchers used a combination of nuclear magnetic resonance diffusion experiments and molecular dynamics simulations to determine the effects of temperature and water on hydrogen-bonding structures in a hydrocarbon (n-heptane surrogate) blended with an oxygenate (ethanol).

At 10% ethanol (all blend percentages are by volume), increasing water content from 2 to 2,000 ppm promoted clustering of the oxygenated species and increased vapor pressure by 5.9% (at 25°C) and 6.5% (at 37.8°C). In contrast, vapor pressure did not change at 50% ethanol because the effects from clustering were overwhelmed by the presence of hydrogen-bonding networks. The results suggest that small differences in water content (or another additive) can influence oxygenate clustering and vapor pressure, offering molecular-level insights into the origins of this behavior that are generally unavailable using thermodynamic ensemble-based modeling approaches.



Plot of ethanol molecules in clusters or hydrogen-bonding networks versus ethanol concentration in n-heptane at 25°C and two water contents. High water content (1,000 ppm) promotes early cluster formation compared with low water content (20 ppm). Vapor pressure is most influenced by water at low ethanol concentrations (0%–10%), but it is effectively insensitive to water once hydrogen-bonding networks form (>30% ethanol). EtOH = ethanol. Figure by Kee Sung Han, Amity Andersen, Richard Overstreet, and Tim Bays, PNNL

CROSSCUTTING STUDY REVEALS REACTIVITY BETWEEN LUBRICANTS AND OXYGENATES

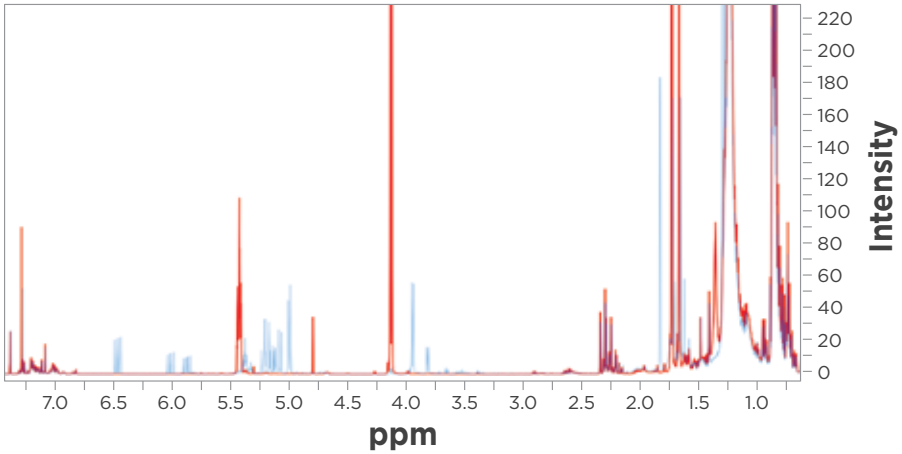
Achievement: A new method that enables rapid assessment of oxygenate-lubricant interactions indicated that three oxygenates—isoprenol, butyl acetate, and 2-ethyl-1-butanol—are likely to be compatible with lubricants.

Potential Impact: This innovative approach to evaluating fuel-lubricant reactivity can identify potential market barriers for new oxygenates, complementing efforts to understand blendstock-fuel system and other engine components' compatibility.

Incompatibility between lubricants and fuels has previously derailed development of new fuels and additives. Co-Optima researchers demonstrated a simple but powerful method to assess oxygenate-lubricant reactivity. Mixtures of a blendstock for oxygenate blending, an oxygenate blendstock, and lubricant components in a lubricant base oil (in a ratio of 5:5:10 by volume) were heated for 2 hours at 150°C in a closed vessel. Lubricant mixtures included base oils blended with an olefin copolymer, polymethacrylates, Molyvan L (a molybdenum-containing friction modifier), ZADP (a zinc-containing anti-wear additive), or a detergent-inhibitor package. The evaluations were also conducted with fully formulated lubricants.

The oxygenates included butyl acetate, isoprenol, prenol, 2-ethyl-1-butanol, and a mixture of polyoxymethylene dimethyl ethers (POMEs) with a polymerization degree ranging from 3 to 6. The specific oxygenates were chosen to span a range of chemical classes studied by Co-Optima. Reactivity was evaluated via gas chromatography using a flame ionization detector (GC-FID) and proton nuclear magnetic resonance (^{1}H NMR) spectroscopy before and after heating.

Spectroscopic data suggested that isoprenol, butyl acetate, and 2-ethyl-1-butanol showed no reactivity with the mixture upon heating, while prenol and POME caused substantial degradation or side reactions, particularly in the presence of lubricant components that contain a metal atom. The same lubricant mixtures did not undergo significant changes in the absence of the oxygenate, indicating that those two oxygenates may be incompatible with the lubricant components. Identification of lubricant-compatible oxygenates can help formulate viable blendstocks.



^{1}H NMR spectra of Molyvan L and prenol before (red) and after (blue) heating at 150°C, showing substantial reactivity evident by peak deviation from original. No reactivity is seen for the Molyvan L/fuel mixture in the absence of oxygenate. Figure by Lelia Cosimbescu, PNNL

MODEL ACCELERATES ACCURATE PREDICTION OF BOND DISSOCIATION ENERGIES, FACILITATES BIOFUEL SCREENING

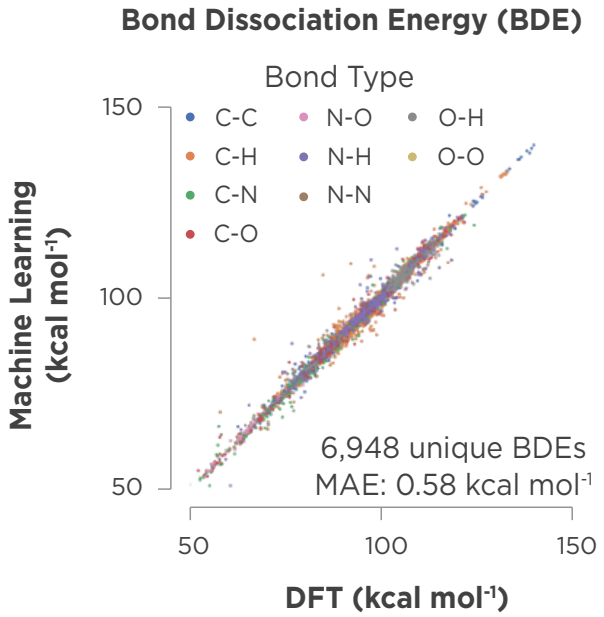
Achievement: A new machine-learning model greatly accelerates BDE calculations for organic molecules.

Potential Impact: Rapidly predicting organic BDEs enables higher-throughput exploration of combustion pathways for new biofuel candidates.

Biofuel combustion is governed by the chemical reactions that each fuel component undergoes. These reaction pathways can lead to the propagation of free radicals that speed autoignition and the production of polycyclic aromatic hydrocarbons that initiate soot formation. Which pathways are favored depends on the chemical structure of the fuels, and the bond dissociation enthalpies (BDEs) of these molecules play a fundamental role in determining which bonds are most likely to participate in chemical reactions. However, BDE computations at the high levels of quantum mechanical theory needed to provide greater accuracy require substantial computing resources.

Because these calculations are slow, BDEs are typically not directly considered for fuel design outside of detailed kinetic mechanism development. To accelerate the computations, Co-Optima researchers constructed a large database of computationally expensive, accurate BDE calculations consisting of 290,664 unique BDEs. The researchers used this database to develop a machine-learning model capable of predicting organic molecule BDEs in a fraction of a second with an accuracy closely rivaling the uncertainty associated with experimental measurements.

A new machine-learning model makes it possible to more rapidly explore potential combustion pathways for previously unstudied molecules. In addition, the speed and accuracy of the BDE predictions enable predicted BDEs to be incorporated into other quantitative structure-property prediction models. For example, incorporating predicted BDEs shows promise for improving predictions of soot formation during combustion of candidate biofuels.



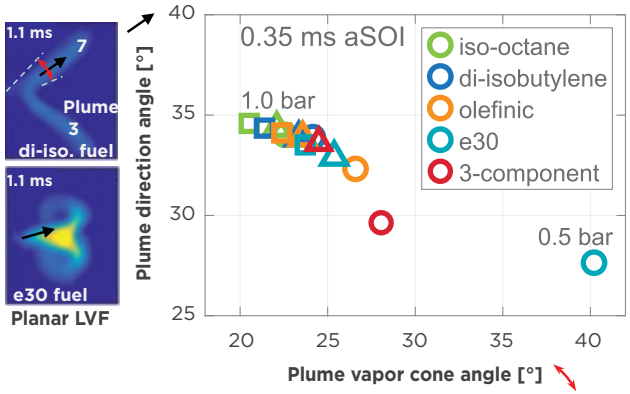
Parity plot showing strong agreement between BDEs from the machine-learning model and highly accurate BDEs calculated via density functional theory (DFT)—with BDE points colored by bond type—resulting in a mean absolute error (MAE) of 0.58 kcal mol^{-1} relative to DFT-calculated values of unseen molecules. Figure by Peter St. John, NREL

UNDERSTANDING FUEL PROPERTY EFFECTS ON PLUME CONE ANGLE LEADS TO BETTER SPRAY DELIVERY

Achievement: A new understanding of the root causes of multi-hole injector spray collapse has been achieved through novel plume-direction and cone-angle measurement techniques.

Potential Impact: Promising fuels may underperform if affected by plume collapse and wall impingement during injection, but collapse can be avoided by injecting at higher gas pressures where plume vapor cone angle remains small.

Understanding how fuel properties affect spray delivery can help develop fuel mixtures better suited for both the boosted SI and ACI modes in multimode engines while avoiding liquid deposits on in-cylinder walls. Co-Optima researchers performed optical extinction imaging in a controlled spray chamber using various fuels and operating conditions corresponding to different injection timings in a multimode engine. Three-dimensional and planar data bisecting plumes of an eight-hole injector were captured by imaging the spray at different rotation angles and then applying computed tomography. When paired with vapor boundary imaging, the technique provided measurements of both the plume direction angle and the vapor plume cone angle. Data obtained over a wide range of operating conditions showed that the plume cone angle essentially dictates the plume direction for multi-hole injectors. For early intake conditions in a vacuum, fuels with significant light-distillate fractions (such as E30, a 30% ethanol blend) have large plumes that quickly merge and collapse to the center, producing poor mixing and liquid wall impingement. Even though E30 has a high octane number and potential for high-efficiency operation, its combustion performance will be degraded if there is liquid impingement. Altering timing to inject into higher charge-gas pressure produces a small plume cone angle and avoids spray collapse, making it feasible to use these fuels with light-distillate fractions that offer superior combustion and efficiency performance.



Direction of individual spray plumes correlates exceptionally well with measured plume cone angle for many fuels and conditions. Symbols indicate ambient pressures (circles = 0.5 bar, triangles = 1.0 bar, and squares = 1.2 bar). Schematics at the left show planar liquid volume fraction (LVF) for an eight-hole injector for two different fuels. aSOI = after start of injection. Figure by Lyle Pickett, SNL

COMPUTATIONAL FLUID DYNAMICS TECHNIQUE ENABLES DETAILED STUDY OF NEAR-INJECTOR TIP DRYING, WITH POTENTIAL FOR SOOT MITIGATION

Achievement: Researchers developed a new computational technique to predict liquid-surface evaporation in high-fidelity computational fluid dynamics simulations of direct fuel injection.

Potential Impact: The tool will inform strategies for reducing soot emissions via injector modifications in conjunction with various fuel blends.

In gasoline direct-injection engines, the prevalent mechanism for forming engine-out soot emissions is linked to deposition and evaporation of liquid fuel in contact with the metal surface. Although cylinder surface wetting can often be controlled through component designs or operating strategies, injector tip wetting is more difficult to avoid. It is therefore crucial to determine how much liquid fuel is deposited and how much evaporates between injection cycles. Co-Optima researchers developed a new technique for predicting liquid-surface regression caused by evaporation in computational fluid dynamics (CFD) simulations of direct fuel injection. At the core of this technique is the efficient separation of the computationally expensive simulation of interphase diffusion, localized at the fuel surface, from the simulation of general diffusion of vapor in air while maintaining mass and energy conservation. The resulting computational tool enables for the first time the study of fuel film interaction with the cylinder's turbulent flow—specifically the evaporation of fuel deposits formed during the injector's closing transient, which has implications for soot formation. Implementation and testing of surface evaporation for single-component fuels was completed in FY20. Ongoing research is focusing on the extension of the technique to multicomponent fuels with composition-dependent evaporation rates.

Capability demonstration in a simulation where iso-octane is injected from a 200-µm pinhole injector. Both liquid surface and vapor concentration are clearly visible in the snapshot; the 1% and 5% vapor mass fractions are rendered by translucent yellow and red iso-surfaces, respectively. Figure by Everett Wenzel and Marco Arienti, SNL

IMPROVED METRIC CHARACTERIZES AUTOIGNITION FOR ACI/SI MULTIMODE ENGINE FUELS

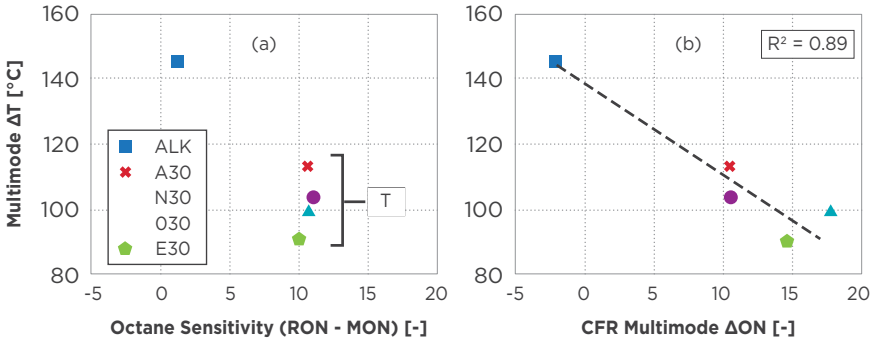
Achievement: Researchers developed a new fuel metric to characterize the autoignition propensity of gasoline fuels for SI multimode and ACI engine operation.

Potential Impact: Accurately characterizing the combined spark-ignited knock resistance and compression-ignited autoignition reactivity of gasoline fuels makes it possible to better specify fuels for multimode LD engines and overcome barriers to efficient ACI combustion.

Gasoline-range fuels for multimode engines must fulfill two seemingly contradictory requirements. ACI operation at part load requires a fuel with high autoignition propensity, while high-load SI operation demands a fuel with high knock resistance (or low autoignition propensity). A theory that fuels with a high RON and low motor octane number (MON) would satisfy these requirements was disproven by previous Co-Optima research, which showed that this was not true for some fuels in ACI mode.

Co-Optima researchers investigated the knock and autoignition propensity of five Co-Optima RON 98 fuels with different chemical compositions. The multimode autoignition propensity was quantified by the intake air temperature required to transition from knock-limited SI to ACI operation. The results showed that although octane sensitivity directionally correlates with the multimode change in intake air temperature, the octane-sensitive fuels exhibit significant intake temperature variations despite having a common octane sensitivity near 10.

The researchers proposed a new ACI-SI multimode fuel metric that uses the octane ratings of the fuels in a CFR engine. Here, a modernized stoichiometric RON test (knock-limited SI) and a MON-like ACI test are used to derive a multimode change in octane number metric. The new results show that change in octane number correlates more strongly with the multimode change in intake air temperature than octane sensitivity does in the LD engine.



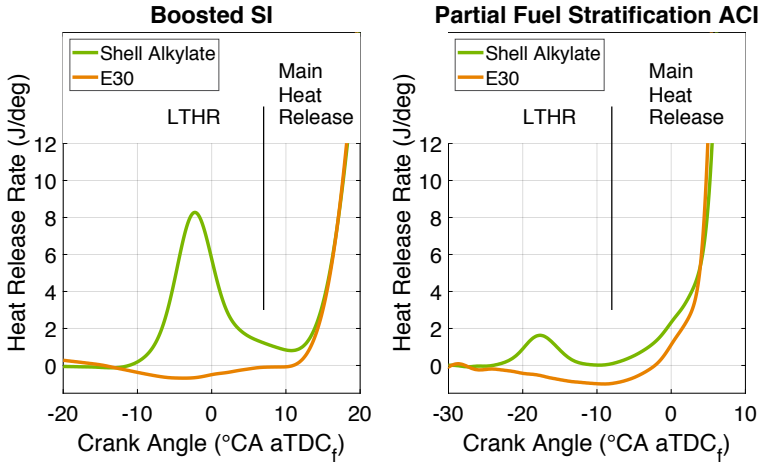
Temperature swing required to switch from knock-limited SI mode to ACI mode in the gasoline direct-injection engine, shown as (a) a function of standard octane sensitivity (RON – MON) and (b) CFR multimode ΔON. The fuels studied include alkylate (ALK), high aromatic (A30), high naphthene/cycloalkane (N30), high olefin/alkene (O30), and high ethanol (E30) fuels. ΔT = change in intake air heating on the multimode engine to switch from knock-limited SI to ACI operation. ΔON = change in octane number based on the critical compression ratio in the CFR engine needed to switch from knock-limited SI to ACI operation. Figure by Toby Rockstroh and Christopher Kolodziej, ANL

UNDERSTANDING THE SPECIFIC ACI MODE EMPLOYED AIDS SELECTION OF OPTIMAL FUELS FOR MULTIMODE ENGINES

Achievement: Research showed two ACI combustion strategies, PFS and SACI, exhibiting LTHR in a similar manner as boosted SI, making fuels with low octane sensitivity promote ACI autoignition—in contrast to previous research showing a homogeneous ACI mode suppressing LTHR so fuels with low octane sensitivity resist ACI autoignition.

Potential Impact: Considering the combustion characteristics of specific ACI modes within multimode strategies will help enable identification of fuels that optimize multimode engine performance.

Co-Optima researchers have targeted identification of fuel properties and compositions to enable high-efficiency multimode combustion by resisting autoignition (or knock) during the boosted SI mode while promoting autoignition during the ACI mode. Research in FY20 suggested there is no single set of desirable fuel properties and compositions, but instead optimal multimode fuel choices are highly dependent on the type of ACI employed. Two ACI combustion strategies—partial fuel stratification (PFS) and SACI—exhibited evidence of LTHR in a similar manner as boosted SI. For SACI, however, the evidence is related to the main autoignition order because the LTHR is obscured by early flame propagation. In both cases, fuels with low octane sensitivity promoted ACI autoignition. In contrast, previous research showed a homogeneous ACI mode suppressing LTHR, so fuels with low octane sensitivity resisted ACI autoignition. Taken together, these results show that understanding the specific ACI mode used to achieve multimode operation is critical in determining the best fuel properties for multimode engines.



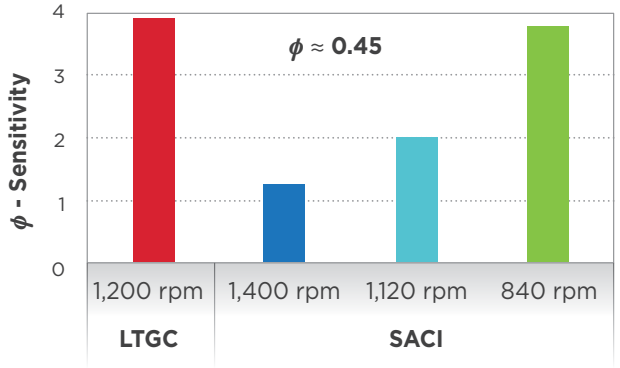
Heat release rates for boosted SI (left) and PFS (right) combustion modes. Both modes exhibit LTHR prior to the main heat release event when a fuel with low octane sensitivity (Shell alkylate) is used, but not when a fuel with high octane sensitivity (E30) is used. °CA aTDCf = degrees crank angle after top dead center firing. Figure by Jim Szybist and Tommy Powell, ORNL

PHI-SENSITIVITY IS INEFFECTIVE FOR ACHIEVING HIGHER LOADS IN SACI COMBUSTION

Achievement: SI engine experiments showed that varying SACI fuel-air stratification produced minor changes in the peak AHRR of autoignition-based combustion when using a phi-sensitive fuel, and chemical kinetics simulations indicated the cause of this weak effect: spark-initiated deflagration happens so fast that the slower ITHR reactions critical to phi-sensitivity have no time to occur.

Potential Impact: The results indicate phi-sensitive fuels do not provide an advantage for SACI combustion.

Phi-sensitivity quantifies how much a fuel's autoignition timing varies with phi (the local fuel/air ratio divided by the stoichiometric fuel/air ratio) within an engine's cylinders. Previous Co-Optima research has shown that fuels with higher phi-sensitivity, combined with fuel stratification, can improve low-temperature gasoline combustion (LTGC), in which ignition is induced by piston compression alone, without any spark. In LTGC, these characteristics can create sequential autoignition that reduces peak heat-release rates and engine knock while enabling higher engine loads. In this latest study, researchers applied a similar approach to an SACI engine using CB#1, a fuel blend previously developed to have increased phi-sensitivity. However, during the SACI experiment, changes to the injection schedules (which varied the fuel stratification) produced only minor changes in the peak apparent heat-release rate (AHRR) of the autoignition-based combustion. Chemkin-Pro modeling revealed that the phi-sensitivity of CB#1 is typically lower for SACI operation than it is for LTGC operation because SACI leaves less time for the intermediate-temperature heat release (ITHR) that is critical to the fuel's phi-sensitivity. The model predicted that the SACI engine speed must decrease to about 840 rpm for CB#1 to achieve the phi-sensitivity that it demonstrates during LTGC at 1,200 rpm. Phi-sensitivity is important for some engine strategies, but it may not provide any benefits for strategies such as SACI that curtail ITHR by accelerating compression to autoignition.



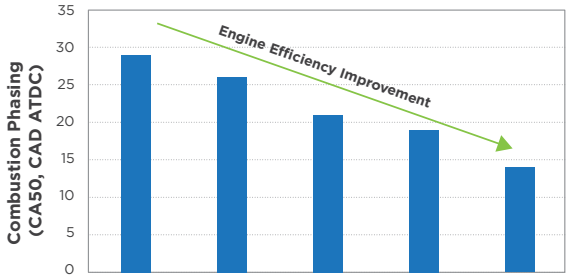
Chemkin-Pro simulation results showing phi-sensitivity (φ sensitivity) vs. engine speed for LTGC and SACI operation. Phi-sensitivity is how much the autoignition time (τ) changes for an incremental change in phi (i.e., −dτ/dφ). Figure by Magnus Sjöberg, SNL

FUELS WITH HIGH OCTANE SENSITIVITY OFFER STRONG PERFORMANCE, EVEN AT HIGH SPEEDS AND LOADS

Achievement: Researchers studied the combination of high RON and high S at high engine speeds and high intake air temperatures to determine impacts on knock-limited engine performance during boosted SI operation.

Potential Impact: For a multimode combustion strategy, increasing S may improve the efficiency of ACI combustion modes at low loads while enhancing the power density of SI combustion at high loads.

Multimode combustion strategies may use ACI at low engine loads to increase efficiency while reverting to boosted SI at high loads to deliver the high power density consumers demand. Increasing the octane sensitivity (S) by lowering the MON and increasing the RON can benefit ACI operation by enhancing the ability to ignite the fuel under high-temperature conditions. However, lower MON may diminish power density at high loads due to onset of engine knock. To clarify this concern, Co-Optima researchers examined potential MON effects at high engine loads and speeds, studying various fuels in a boosted SI engine with a compression ratio of 12.4. Researchers found that—even at 4,000 rpm—fuels with a RON of at least 97 and high S (>10) allowed the knock-limited combustion phasing (CA50, the crank angle at which 50% of the fuel has burned) to be advanced by up to 8 crank angle degrees (CAD) compared with iso-octane (RON = 100, S = 0). The advanced combustion phasing translates into greater engine efficiency and higher torque. A related chemical kinetic modeling study showed that increasing S should continue to be beneficial at speeds up to 6,000 rpm and at elevated intake temperatures up to 100°C. These findings demonstrate that increasing S while retaining a target RON value should improve ACI operation at low loads, as well as SI operation at high loads.



	Isooctane	Co-Optima Aromatic	Diisobutylene Blend	Co-Optima E30	E20 Blend
RON	100	98.0	98.2	98.3	101.3
MON	100	87.3	88.0	87.6	88.8
S	0	10.7	10.2	10.7	12.5

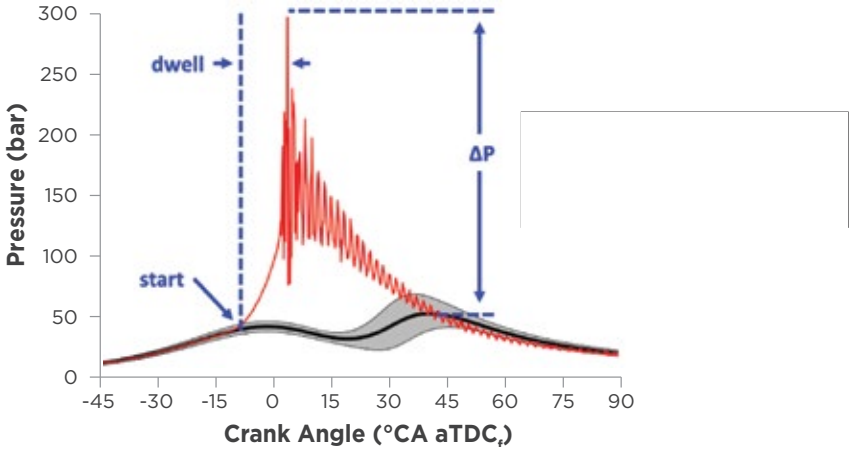
Boosted SI knock-limited combustion phasing for fuels with various chemistries and S values. Compared with iso-octane (S = 0), fuels with high S enabled more advanced combustion phasing and higher efficiency at 4,000 rpm and 16-bar brake mean effective pressure (BMEP) conditions. Different fuel chemistries produced different CA50 phasing at the same S, indicating the importance of chemical kinetics during the combustion process. ATDC = after top dead center. Figure by Scott Sluder, ORNL

CORRELATION SHOWS EFFECTS OF PMI ON LSPI AND ENGINE EFFICIENCY

Achievement: Using a unique approach based on the Co-Optima merit function, researchers captured data on reduced efficiency associated with LSPI and fuel PMI in downsized boosted SI engines.

Potential Impact: Understanding the relationships between LSPI, PMI, and efficiency could facilitate engine downsizing and downspeeding, leading to higher engine efficiency, lightweighting, and improved vehicle fuel economy.

Engine downsizing and downspeeding can deliver higher engine efficiency, lightweighting, and improved vehicle fuel economy. However, low-speed pre-ignition (LSPI) poses barriers to these technologies because its occurrence results in catastrophic premature engine failures and limits engine downsizing potential. Co-Optima researchers analyzed existing engine data to understand how LSPI limits engine efficiency. They discovered a correlation between fuel particulate matter index (PMI) and LSPI and integrated the LSPI and PMI results into the Co-Optima merit function, which is used to quantify the impact of fuel properties on SI engine efficiency. This analysis showed that LSPI, and hence PMI, limit the efficiency benefits that can be obtained from other fuel properties such as RON, S, and heat of vaporization. The finding demonstrates how a single fuel property, PMI, originally developed to characterize emissions propensity, can affect several secondary aspects of engine efficiency. The fact that PMI is correlated with LSPI also implies that a fuel's LSPI propensity is related to the presence of high-boiling-point aromatic compounds. This novel approach is currently being investigated for applicability to multimode engines and for exploring further connections between PMI, LSPI, and efficiency.



Example of cylinder pressure measurements for normal combustion and LSPI that can result in catastrophic engine damage and failure. P = pressure, SD = standard deviations. Figure by Derek Splitter, ORNL

KINETIC MODEL VALIDATED FOR BLENDS OF ISO-OCTANE WITH NITRIC OXIDE, IMPROVING SIMULATIONS OF EGR EFFECTS ON AUTOIGNITION

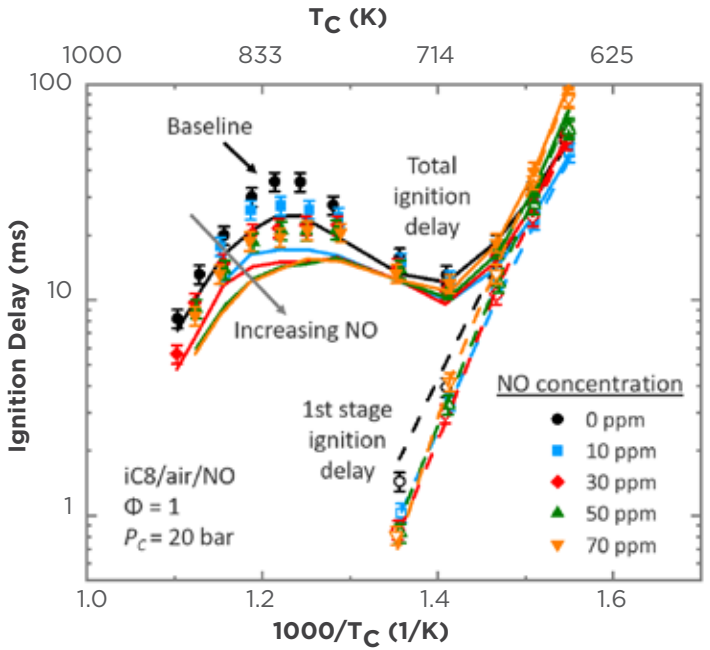
Achievement: Researchers validated the Co-Optima chemical kinetic model for iso-octane blended with trace amounts of NO.

Potential Impact: Improving the accuracy of kinetic models is important for predicting EGR effects on autoignition in engine simulations, which can accelerate advanced engine development.

Exhaust gas recirculation (EGR), which feeds some of an engine's exhaust back into the engine cylinders, reduces engine-out nitrogen oxides (NO_x) emissions and can increase engine efficiency. Among the key components of recirculated exhaust, nitric oxide (NO) is known to have the largest effect on ignition timing.

Researchers validated the Co-Optima chemical kinetic model for iso-octane (a simple gasoline surrogate) blended with trace amounts of NO. Combustion reactions relevant to NO and iso-octane were incorporated into the model by combining existing kinetic mechanisms from the scientific literature with additional reaction classes derived from studies of n-pentane combustion with NO or nitrogen dioxide (NO_2). Predictions of ignition delay time as a function of the temperature of iso-octane blended with 0–70-ppm NO were compared with experiments performed in a rapid compression machine.

The researchers found strong agreement between the modeled and experimental results, with 90% of the simulated values within a factor of 1.5 of the corresponding experimental values. Accurately incorporating the relevant chemical reactions into a kinetic model helps correctly predict combustion behavior in engines. Prediction of ignition promotion and inhibition due to NO has important implications for controlling engine knock in boosted SI engines and controlling combustion phasing in multimode and ACI engines.



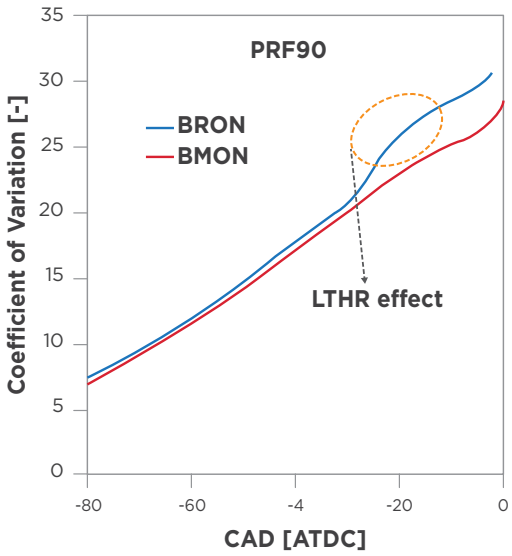
Ignition delay time vs. engine-cylinder temperature (T_C) for blends of NO in iso-octane, derived from kinetic modeling (lines) and rapid compression machine experiments (symbols). Error bars represent ±10% of mean experimental measurements. iC8 = iso-octane; Φ = equivalence ratio; P_C = pressure after end of compression (at top dead center). Figure by Chiara Saggese, LLNL, and University of Connecticut

CFD MODEL REVEALS IMPLICATIONS OF LOW-TEMPERATURE HEAT RELEASE FOR ACI CONTROL

Achievement: Simulated HCCI engine operation showed greater thermal stratification due to LTHR under BRON conditions than under BMON conditions, producing the longer combustion duration characteristic of enhanced sequential autoignition.

Potential Impact: ACI may be more controllable in practical engines under BRON conditions than under BMON conditions.

Multimode engine operation is hindered by uncontrolled autoignition with excessively high pressure-rise rates in the ACI mode. One potential approach to mitigate this issue is using LTHR to create temperature gradients in the fuel-air charge, leading to sequential autoignition and heat release spread over a longer time. Co-Optima researchers explored use of LTHR for ACI control by simulating homogeneous-charge compression-ignition (HCCI) combustion of a PRF gasoline surrogate with RON and MON of 90. The simulations were performed using a CFD model of the CFR engine under "beyond RON" (BRON) conditions (higher pressure than standard RON conditions) and "beyond MON" (BMON) conditions (higher temperature than standard MON conditions). The CA50 was held constant by adjusting the compression ratio. The simulation results showed that the exclusive occurrence of LTHR under BRON conditions enhanced in-cylinder temperature stratification, producing longer combustion duration (CA10 – CA50) compared with the duration under BMON conditions. This longer combustion duration is characteristic of enhanced sequential autoignition, suggesting that ACI operation under BRON conditions may be better suited for practical engines than operation under BMON conditions.



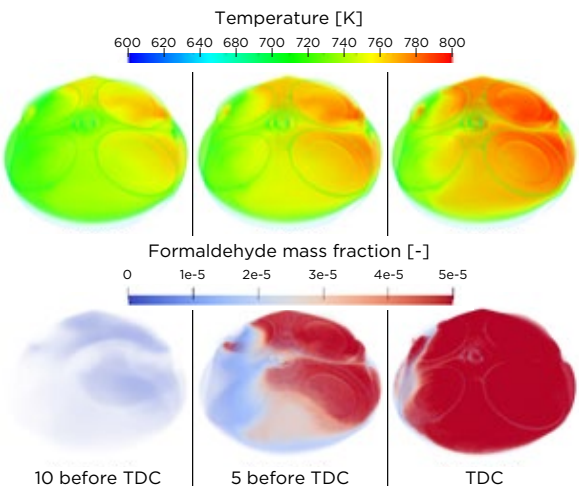
Temporal evolution of temperature stratification expressed in terms of coefficient of variation (the ratio of the standard deviation to the mean value of in-cylinder temperature) up to CA10 (the crank angle at which 10% of the fuel is burned). CFD simulations performed using the virtual CFR engine model are for PRF90 under BRON and BMON ACI conditions at the same CA50 of 3 CAD ATDC (global equivalence ratio = 0.3, engine speed = 600 rpm). The combustion duration (CA10 – CA50) is 5.66 CAD for BRON conditions and 2.8 CAD for BMON conditions. Figure by Pinaki Pal, ANL

COMPUTATIONAL MODEL REVEALS THE DYNAMICS OF PRE-SPARK HEAT RELEASE

Achievement: A first-of-its-kind study characterized low-temperature PSHR using a new three-dimensional CFD model, dramatically improving the understanding of this phenomenon.

Potential Impact: Accurate PSHR simulations improve predictions of engine knock and can help control it.

LTHR in spark-ignited internal combustion engines is a necessary step in the autoignition process known as engine knock, which can adversely affect engine performance and reliability. Accurate LTHR predictions are fundamental to understanding and controlling the knock phenomenon. LTHR is typically obscured by the deflagration following spark ignition, but extremely late ignition timing can lead to LTHR before the spark, known as pre-spark heat release (PSHR). Co-Optima researchers developed and validated a three-dimensional CFD model that shows PSHR beginning in the fuel-lean region of an engine cylinder but exhibiting higher intensity in the fuel-rich region. The superimposition of the in-cylinder pressure-temperature trajectories on the first-stage and main ignition delay maps revealed PSHR's influence on engine knock and demonstrated the effect of fuel properties (such as laminar flame speed and heat of vaporization) on PSHR's timing and intensity. Predictions based on two fuels and several engine operating conditions indicated that trapped in-cylinder residuals from the previous cycle's incomplete combustion have a strong impact on PSHR. For a given engine platform, this new computational tool can provide quick evaluations of fuel effects and the corresponding in-cylinder thermodynamics of PSHR, which will help clarify the causes of knock.



Simulation using the new computational model of boosted SI engine operation with Co-Optima alkylate fuel as the piston approaches top dead center (TDC). At 10 CAD before TDC (left column), stratification of temperature and equivalence ratio (not shown here) is observed, with the area near the intake valves being generally warmer and leaner. Between 10 and 5 CAD before TDC, low-temperature reactions start occurring, resulting in higher temperatures and initial generation of formaldehyde (center column). At TDC, PSHR reaches its maximum, with broader temperature increases and intense formaldehyde production. Spark ignition is finally set to occur at 6 CAD after TDC. Figure by Hengjie Guo and Roberto Torelli, ANL

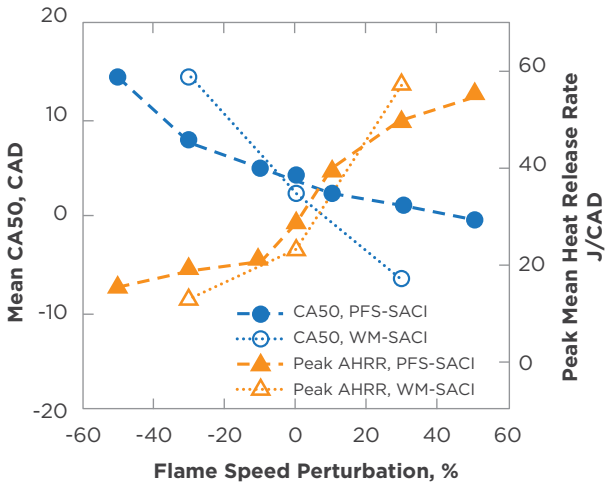
Photo: ORNL

MODEL PREDICTS FLAME-WALL INTERACTION AND FUEL PROPERTY SENSITIVITIES IN SACI ENGINES WITH AND WITHOUT PARTIAL FUEL STRATIFICATION

Achievement: A high-fidelity computational model for PFS-assisted SACI—which considered flame-wall interaction and agreed with experiments and first-principles simulations—was used to quantify fuel-property impacts on SACI operation with and without PFS.

Potential Impact: The model provides new insights into fuel-property impacts on SACI multimode engine operation.

The PFS fuel-injection strategy holds potential to significantly increase the reliability of SACI—a promising multimode approach—by improving combustion stability and subsequently reducing cycle-to-cycle variability under lean or dilute conditions. Co-Optima researchers developed a computational model based on large-eddy simulations that enables high-fidelity multicycle investigation of PFS-assisted SACI with improved flame-wall interaction treatment. The model agreed with experiments in terms of global quantities (such as pressure and heat-release rate traces) and local quantities (such as the spatial distribution of deflagration vs. autoignition). The model also captured the triple-flame structure that drives initial combustion in stratified mixtures, as verified by a first-principles simulation using Nek5000 (a spectral element code). Most importantly, the researchers used the model to identify key differences in fuel-property impacts between PFS-assisted SACI and well-mixed (no PFS) SACI when spark timing was fixed. Despite similar responses across the two SACI modes to perturbations in the fuel's heat of vaporization, results suggest that PFS-assisted SACI was less affected by perturbations in the fuel's laminar flame speed than well-mixed SACI. These findings demonstrate the pivotal role of PFS in stabilizing lean or dilute SACI combustion.



Impacts of laminar flame speed on CA50 combustion phasing and peak mean heat release rate (AHRR, in joules per CAD) for SACI engine operation with PFS (PFS-SACI) and without PFS (WM-SACI) under fuel-lean conditions, predicted by multicycle CFD simulations. Figure by Chao Xu, ANL

AUTOMATICALLY GENERATED KINETIC MECHANISM REVEALS CRITICAL PYROLYSIS PATHWAYS IN BIOFUEL COMBUSTION

Achievement: As part of combustion mechanism development, detailed kinetic mechanism for high-temperature cyclopentanone pyrolysis was developed using automated software and validated via experimental data, revealing the significance of previously neglected radical-involved pathways.

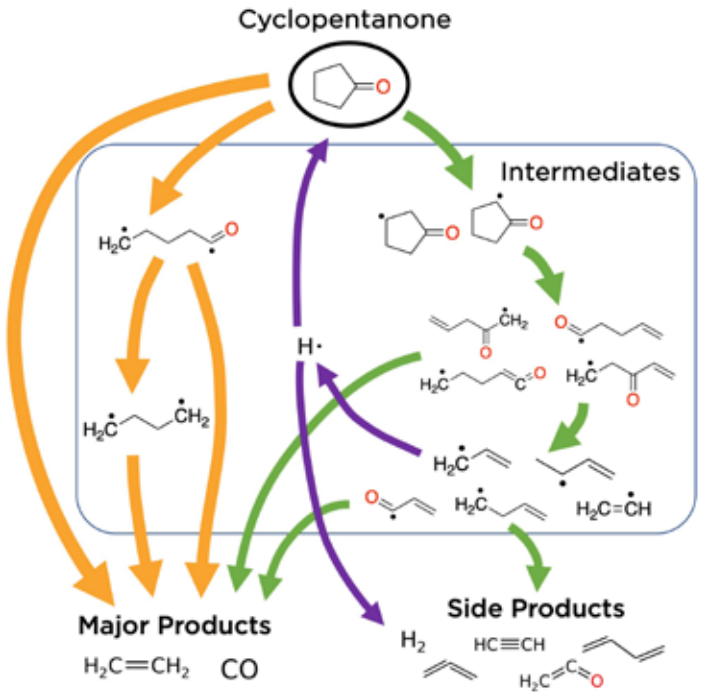
Potential Impact: The study helps clarify biofuel pyrolysis chemistry, increasing the accuracy of and decreasing the time required for fuel property and combustion predictions made by automated computer programs to help guide decisions about commercial development of new biofuels.

High-fidelity kinetic mechanisms—parametrized models indicating the microscopic transformations and pathways from reactants to products—play essential roles in understanding fuel properties and conducting engine simulations for fuel-engine co-optimization. However, the long turnaround time and limited adaptability caused by mechanism incompleteness and inaccurate parameters in conventional model generation hinder the application of kinetic mechanisms for evaluating new biofuels at large scales.

Co-Optima researchers demonstrated use of the automated Reaction Mechanism Generator (RMG) software to develop a detailed mechanism for high-temperature pyrolysis of cyclopentanone, a potential biofuel component. With a machine-learning-based parameter-acquisition algorithm and an advanced rate-based model-enlarging algorithm, RMG can generate comprehensive kinetic models at significantly reduced cost compared with conventional methods.

The RMG-generated cyclopentanone mechanism includes important unimolecular pathways reported by other studies while identifying the significance of radical-involved pathways that were previously neglected. This new mechanism was validated by comparing simulated results, including species time histories and branching ratio, against experimental data from a shock tube.

The results fill the gap in understanding cyclopentanone pyrolysis chemistry and inform pyrolysis and combustion models for other biofuels. Ultimately, the study will increase the accuracy of automated computer programs' fuel property and combustion predictions and help guide decisions about commercial development of new biofuels.



Dominant reaction pathways of cyclopentanone pyrolysis at high temperature. The unimolecular pathways are colored orange, and radical-involved bimolecular pathways are indicated by green and purple. Figure by William Green and Xiaorui Dong, MIT

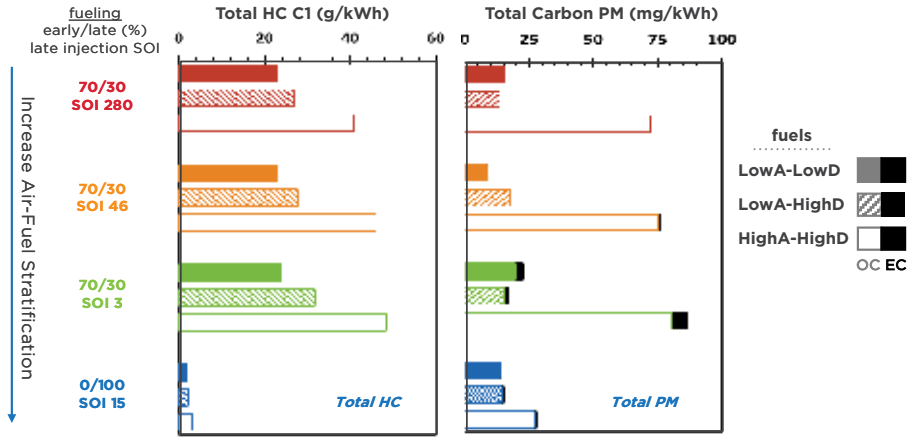
FUEL AROMATIC CONTENT AFFECTS EMISSIONS MORE THAN FUEL VOLATILITY ACROSS ACI MODES FOR MULTIMODE ENGINES

Achievement: Researchers demonstrated that higher aromatic content in gasoline-range fuels has a more significant impact than fuel distillation range on engine-out PM and HC emissions across several ACI modes.

Potential Impact: The research answered a critical question relevant to the composition of fuels that exhibit lower emissions in ACI combustion.

Co-Optima researchers demonstrated that the chemical (aromatic content) and physical (distillation range) properties of gasoline-range fuels can change the amount of engine-out particulate matter (PM) and hydrocarbon (HC) emissions across several ACI modes. By isolating the impact of fuel aromatic content or distillation range, the researchers found that both influence PM and HC emissions, but increases in aromatic content typically result in greater emissions across the entire range of ACI modes studied.

ACI strategies can be combined with other engine modes, such as boosted SI, to improve efficiency under a range of operating conditions. However, the diversity of combustion approaches used in multimode engines—as well as the range of chemical and physical properties of potential fuels designed for these engines—may present novel emissions-control challenges. A fundamental understanding of engine-out emissions during ACI operation is needed to ensure that future light-duty vehicles employing multimode engines can cost-effectively meet emissions regulations.



Total HC (left) and total carbon PM (right) emissions as a function of ACI mode in an LD engine. Vertical axes are color coded and given as early injection fraction/late injection fraction, with the start of injection (SOI) for the early fuel injection always at 280 CAD before top dead center (bTDC) and late SOI listed in CAD bTDC at constant combustion phasing. Low aromatic (LowA) = 7–8 vol % aromatic content; high aromatic (HighA) = 26 vol % aromatic content; low distillation (LowD) = 189°F–253°F distillation temperatures (T50–T90); high distillation (HighD) = 246°F–343°F distillation temperatures (T50–T90); EC = elemental carbon; OC = organic carbon; T50 = temperature at which 50% of the fuel evaporates. Figure by Melanie Moses DeBusk, ORNL

HIGH-PERFORMANCE BLENDSTOCKS MITIGATE MULTIMODE ENGINE EMISSIONS-CONTROL CHALLENGES

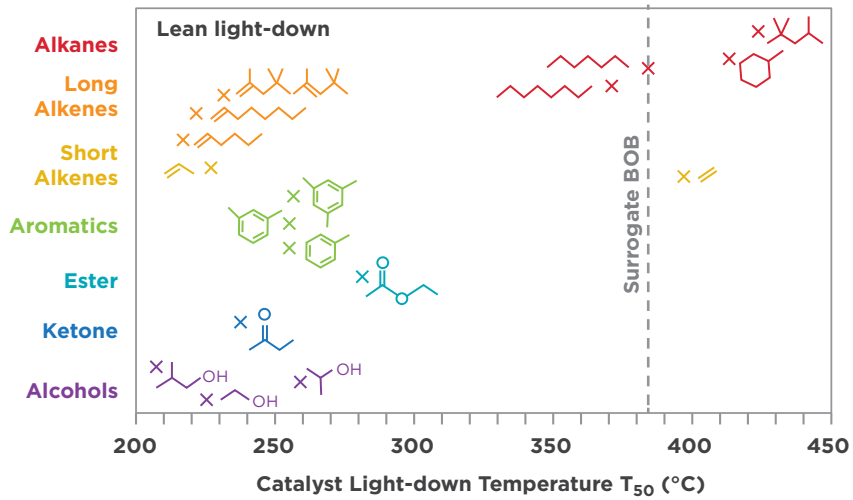
Achievement: Researchers quantified differences in the catalytic reactivity of a surrogate BOB and 15 high-performance blendstocks under lean and stoichiometric conditions.

Potential Impact: Although both stoichiometric (SI mode) and lean (ACI mode) conditions must be considered when evaluating potential multimode engine emissions, the increased reactivity of high-performance blendstocks under ACI conditions could offer emissions-control benefits.

Multimode gasoline-fueled engines—using stoichiometric SI combustion during cold start and at high loads and switching to ACI combustion at low loads—offer higher fuel efficiency than conventional engines. However, multimode engines introduce emissions-control challenges. For example, during the switch from high-load SI to low-load ACI operation, exhaust composition abruptly changes from stoichiometric to lean and exhaust temperatures drop rapidly. Such operating conditions could impact three-way catalyst (TWC) efficiency that mitigates regulated emissions.

To quantify fuel chemistry effects on multimode engine TWC performance, Co-Optima researchers measured the stoichiometric "light-off" temperature (at which the TWC begins converting pollutants effectively) and the lean "light-down" temperature (below which the TWC stops converting pollutants effectively) for 15 high-performance blendstocks and a surrogate BOB over a commercial TWC in a flow reactor. Reactivity trends under stoichiometric light-off and lean light-down varied significantly with chemical structure, highlighting the need to evaluate the reactivity of potential blendstocks in both operating modes.

The lower lean light-down temperatures of the high-performance blendstocks—especially the alcohols—relative to the less-reactive alkanes that dominate petroleum-based gasoline blends could make it easier for multimode engines to achieve emissions compliance when using the high-performance blendstocks. The results also suggest the possible need to tailor catalysts to multimode engines.



Fuel lean light-down temperature for 15 of the high-performance blendstocks, two short alkenes commonly found in exhaust, and the surrogate BOB (55% iso-octane, 25% toluene, 15% n-heptane, and 5% 1-hexene) over an aged commercial TWC under ACI-relevant conditions. From bottom to top, the pure fuel species shown are ethanol, isopropanol, isobutanol, 2-butanone, ethyl acetate, toluene, m-xylene, mesitylene, ethene, propene, 1-hexene, 1-octene, diisobutylene, n-heptane, n-octane, methylcyclohexane, and iso-octane. For each blendstock, "X" represents T50: the temperature at which 50% of the fuel species were converted by the TWC. Figure by Sreshtha Sinha Majumdar, ORNL

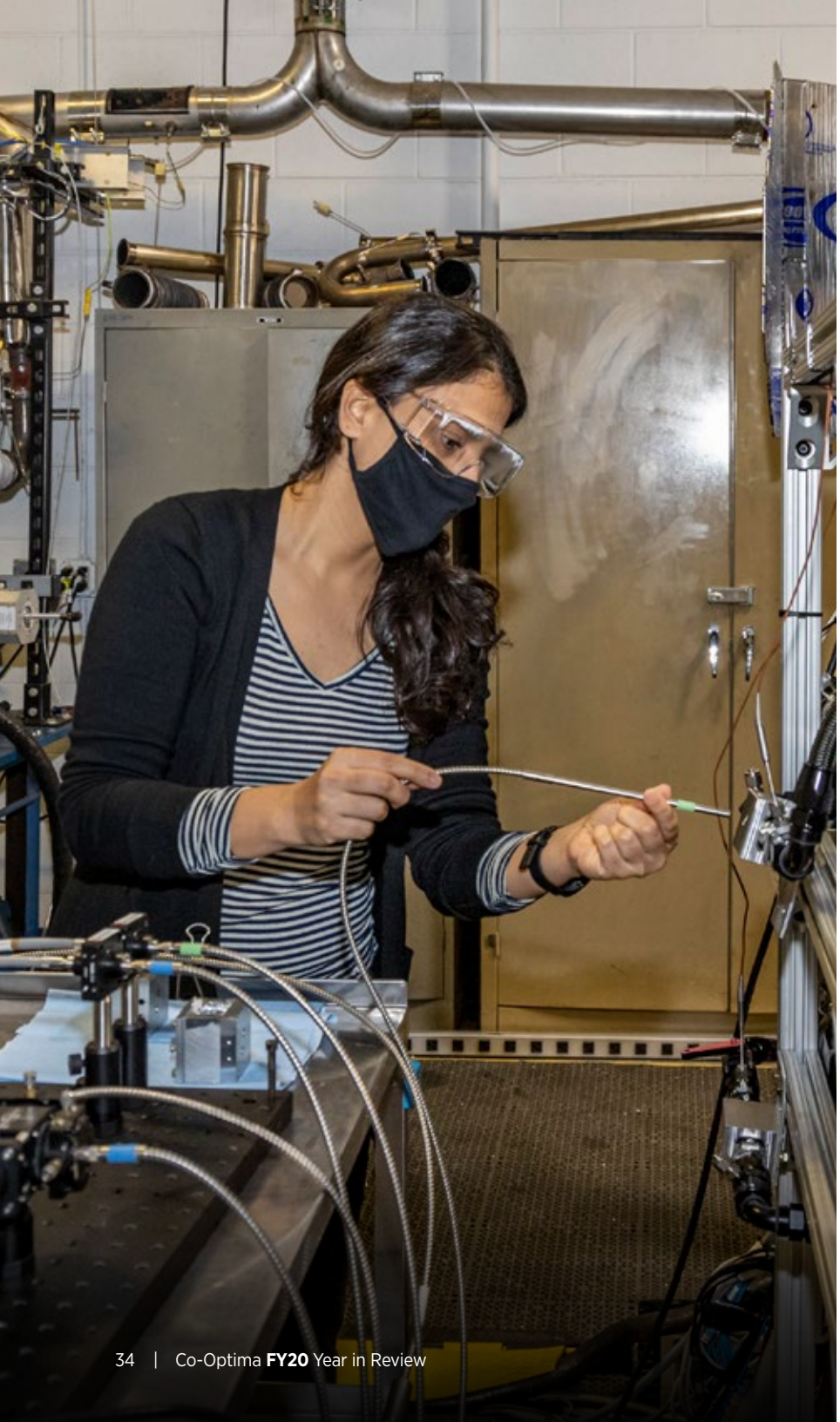


Photo: ORNL

GHG-ADVANTAGED BIOBLENDSTOCK CANDIDATES FOR MULTIMODE ENGINES VARY BY PROJECTED COST AND TECHNOLOGY READINESS

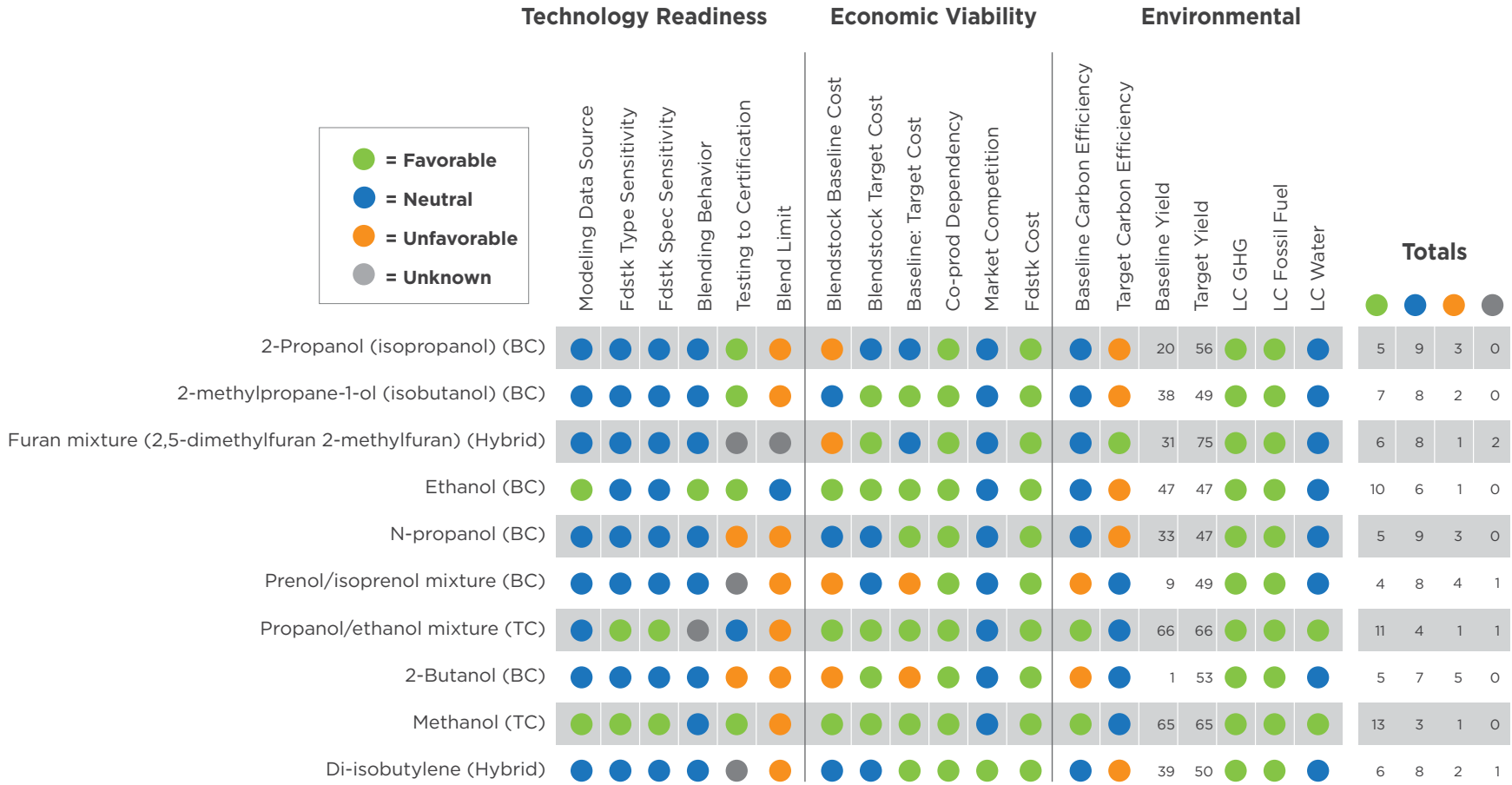
Achievement: Researchers analyzed the technology readiness, economic viability, and environmental impact of 10 bioblendstock candidates with potential for use in multimode engines, all of which provide synergistic octane blending, GHG emissions reductions greater than 60%, and volumetric cost performance parity with gasoline.

Potential Impact: The analyses help gauge prospects for commercial-scale displacement of conventional gasoline use in multimode engines with bioblendstock use, while focusing fuels research and development on improvements that provide the greatest benefits.

Co-Optima researchers used techno-economic and life cycle analyses to assess 19 metrics for technology readiness, economic viability, and environmental impact across 10 bioblendstock candidates with potential for use in multimode engines. These candidates were selected because they can offer synergistic octane blending and the potential to reduce life cycle GHG emissions by at least 60% compared with conventional gasoline. Most process-modeling data sources were based on bench-scale data, making evaluation of commercial-scale impacts more uncertain, although ethanol and methanol have been demonstrated at commercial scales.

The biochemical pathways are moderately sensitive to variations in biomass feedstock type and quality (in relation to feedstock carbohydrate content and biomass recalcitrance). Although most candidates contain alcohol functional groups, many of which are approved fuel additives, current regulations limit the volumes of most candidates that could be blended with gasoline.

When normalized by energy content, the economic viability results showed potentially competitive target costs: less than $4 per gasoline gallon equivalent (GGE) for most candidates, and less than $2.5/GGE for methanol. In addition, the corn stover and woody biomass feedstocks used to produce the bioblendstocks can be obtained at reasonable costs and in quantities required for large-scale deployment, although competition for these feedstocks from other markets may put pressure on cost, availability, or both.



Techno-economic and life cycle analysis results for selected multimode bioblendstock pathways, categorized and compared based on favorability for each metric. Routes generally do not include coproducts. Feedstock costs, as well as life cycle impacts on GHG emissions and fossil fuel and water consumption, represent comparison to a future target case. Favorable, neutral, and unfavorable thresholds for each category were set in consultation with conversion and fuel experts. Baseline and target yields are expressed in GGE per dry U.S. ton. BC = biochemical, co-prod = co-production, Fdstk = feedstock, LC = life cycle, spec = specification, TC = thermochemical, Hybrid = biochemical conversion of biomass with TC upgrading step. Figure by P. Thathiana Benavides (ANL) and Andrew Bartling (NREL), with contributions from Steven Phillips (PNNL), Troy Hawkins (ANL), and Avantika Singh (NREL)

Photo: ORNL

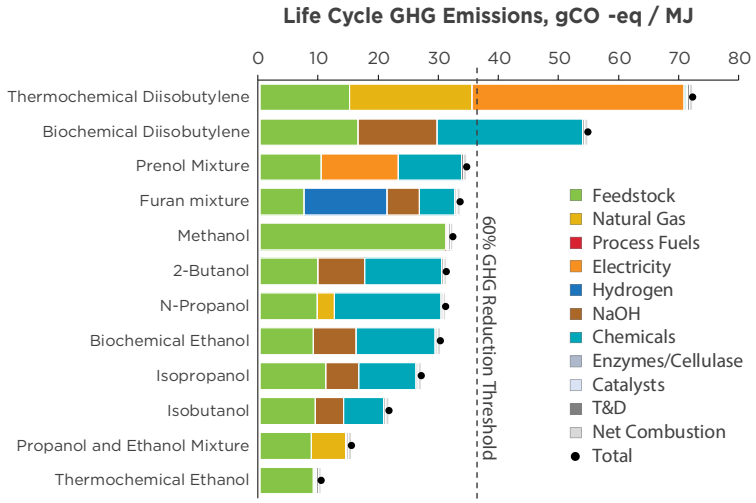
ANALYSIS IDENTIFIES NINE PROMISING MULTIMODE BIOBLENDSTOCKS THAT CAN REDUCE LD GHG EMISSIONS BY UP TO 89%

Achievement: Life cycle GHG results were compared for 10 bioblendstocks that could enable co-optimization of multimode engines and fuels.

Potential Impact: Life cycle analysis helps identify blendstocks and production pathways with the greatest potential for reducing emissions.

Co-Optima researchers assessed the life cycle GHG emissions of 12 pathways to 10 promising bioblendstocks identified as enabling co-optimization for multimode engine configurations. This assessment, especially at early stages of research, provides a natural feedback loop to inform process design and guide the development of sustainable fuels. The life cycle GHG emissions were evaluated using Argonne National Laboratory's 2020 GREET (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) model.

Life cycle GHG emissions ranged from 10 to 72 g of CO_2 equivalent per megajoule (gCO_2e/MJ) across the bioblendstocks, with the sources of GHG emissions varying substantially. Overall, the analysis showed feedstocks, electricity, hydrogen, and sodium hydroxide as the primary contributors to GHG emissions. Of the 10 bioblendstocks examined, nine blendstocks showed potential to reduce GHG emissions by 62% to 89% relative to a baseline petroleum gasoline.



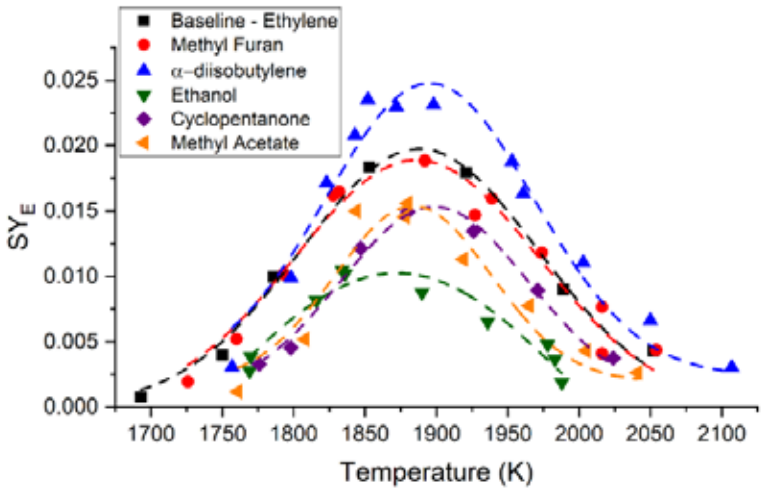
Life cycle GHG emissions for multimode blendstock candidates showing contributions from feedstocks, conversion (energy and other inputs like sodium hydroxide and hydrogen), and fuel use. Results are benchmarked against a 60% GHG reduction target relative to baseline petroleum fuels (vertical dashed line). Figure by George G. Zaimes with contributions from P. Thathiana Benavides and Troy Hawkins, ANL

SHOCK-TUBE STUDY REVEALS THE IMPACT OF BIOFUEL BLENDING ON SOOT EMISSIONS UNDER ENGINE-RELEVANT CONDITIONS

Achievement: Shock-tube/laser-extinction experiments evaluated the impact of biofuel blends on soot formation at high temperature.

Potential Impact: The results inform the development of soot formation kinetic simulations of biofuel blends that can provide emissions benefits.

Biofuels can be blended with conventional fuels because of similarities in composition and other physical and chemical properties, but this blending can have a significant impact on emissions. Co-Optima researchers used shock-tube experiments coupled with a nonintrusive laser-extinction technique to simulate engine conditions and quantify the amount of soot formed from biofuel blends at high temperatures (1,700–2,100 K) and 4–4.7 atm of pressure. Mixtures of 75% ethylene and 25% bioblendstock were prepared, maintaining a constant atomic carbon content of 5% and equivalence ratio of 8.6. Results revealed that the ethanol blend formed the least soot, while the α-diisobutylene blend produced more soot than the baseline (100% ethylene) mixture. These experimental data inform the development of biofuel blends that can provide emissions benefits.



Soot yield x E(m) (SY_E) vs. temperature at 1.5 ms for blends of 75% ethylene and 25% indicated bioblendstock, as measured in shock-tube experiments. The baseline fuel is 100% ethylene. Lower SY_E indicates lower soot emissions. E(m) is a function of soot refractive index. Figure by Ramees Rahman and Subith Vasu, University of Central Florida

Photo: NREL

BLENDING OPTIMIZATION ANALYSIS LINKS PROPERTIES OF GASOLINE-RANGE BIOBLENDSTOCKS WITH THEIR POTENTIAL VALUE TO PETROLEUM REFINERS

Achievement: Blending optimization showed the correlation between the properties of gasoline-range bioblendstocks and the economic value of the bioblendstocks to refiners; octane was especially important for economic value, in addition to vapor pressure, which is more strictly regulated in summer.

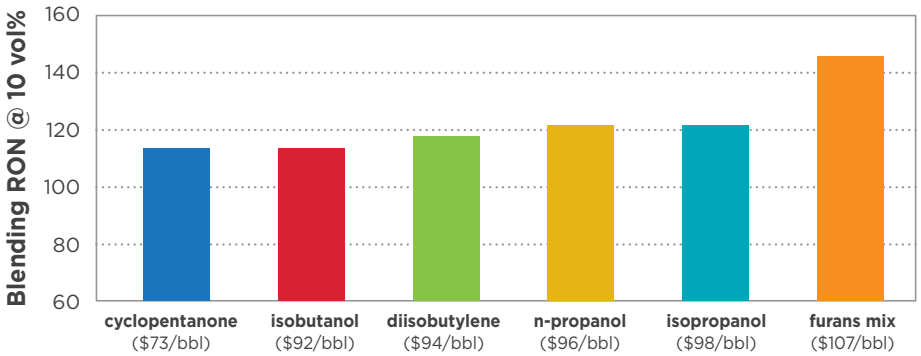
Potential Impact: The results identified market opportunities for additional value that could be derived from bioblendstocks.

Co-Optima researchers quantified the breakeven value of six gasoline-range bioblendstock candidates to petroleum refiners at $73 per barrel (bbl) to $107 per bbl based on analytical tools and methods used in the petroleum industry. The results indicate that the bioblendstock RON has the largest impact on value.

The breakeven value in this petroleum-blending operation is defined as the maximum purchase cost of a bioblendstock that would deliver the same specification in the finished gasoline and maintain the same profitability. This value arises from the superior properties of bioblendstocks—such as high octane number, high octane sensitivity, and low Reid vapor pressure (RVP)—which refiners can exploit to meet commercial fuel specifications at costs lower than could be achieved using petroleum streams alone.

The researchers first developed nonlinear property blending models in Aspen PIMS, planning software used widely by refiners to maximize refinery gross margin. These models used Co-Optima experimental measurements quantifying blending effects on final fuel properties, including RVP, RON, MON, and distillation temperatures at which 10%, 50%, and 90% (by volume) of the fuel evaporates. The models were applied to optimize blending to maximize plant economic benefits, subject to fuel property constraints, especially octane number and RVP.

In addition, for bioblendstocks with a low boiling point such as isopropanol, the final blend might be constrained by T50 (the temperature at which 50% of the fuel evaporates) at a high blend level. For bioblendstocks with a high boiling point, such as diisobutylene, T10 (temperature at which 10% of the fuel evaporates) might become an important property constraint. Finally, the values of the bioblendstocks to petroleum refiners were derived from the difference in plant economics with and without adding the bioblendstocks. Ultimately, refiners could derive additional value using the higher octane and lower vapor pressure to meet fuel specifications.



Blending RON—at 10% by volume in E0 (gasoline with zero ethanol content)—vs. breakeven values of bioblendstocks to petroleum refiners, showing a largely monotonic increase in value with increasing RON. Breakeven values are determined by the gasoline blending operation. Pricing is based on averages for 2013–2017. Figure by Yuan Jiang, PNNL

Medium- and Heavy-Duty Fuel and Engine Research

MCCI and ACI Breakthroughs: Combining Diesel Efficiency with Fewer Emissions

The Co-Optima team is working to improve medium-duty (MD) and heavy-duty (HD) engine efficiency and maintain fuel energy density while making emissions compliance more affordable through research spanning mixing-controlled compression ignition (MCCI) and advanced compression-ignition (ACI) combustion approaches.

The combination of MCCI combustion's high thermal efficiency and torque with diesel-range fuels' high energy density delivers the power and fuel economy needed for most of the commercial freight trucks found on today's roads. However, these engines require costly and complex control systems to meet emission regulations.

Because diesel engines are already highly efficient, there is only modest potential to further increase efficiency. This means that Co-Optima's primary strategy for MD/HD trucks is to identify new blendstocks and engine technologies that improve economic and environmental impacts. Fuels that produce less nitrogen oxide (NO_x) and soot emissions may also help reduce MCCI engine operating costs. Under certain conditions, fuels with different properties than conventional diesel may make it possible to use advanced combustion modes that deliver greater efficiency and even fewer emissions.

Fiscal Year 2020 (FY20) Co-Optima MCCI research has included analyses of the economic and environmental potential of new fuels, as well as engine combustion research revealing how these fuels affect the NO_x-particulate matter (PM) trade-off. Researchers combined bioderived oxygenate fuels with ducted fuel injection (DFI) to demonstrate its promise as an advanced MCCI strategy capable of providing high efficiency along with low NO_x and soot emissions.

ACI, which includes low-temperature combustion approaches such as mixed and partially stratified compression ignition paired with gasoline-range fuels, has the potential to simultaneously deliver high thermodynamic efficiencies and low emissions. Co-Optima researchers have dedicated significant efforts to pinpointing fuel properties that affect ignition delay-time sensitivity to phi (fuel-to-air equivalence ratio), which will be crucial to expanding ACI load range. Advanced control strategies for operations, including fuel stratification, injection, and dilution, have also been important focus areas.

Select Co-Optima accomplishments related to MD and HD vehicles can be found in the following section.

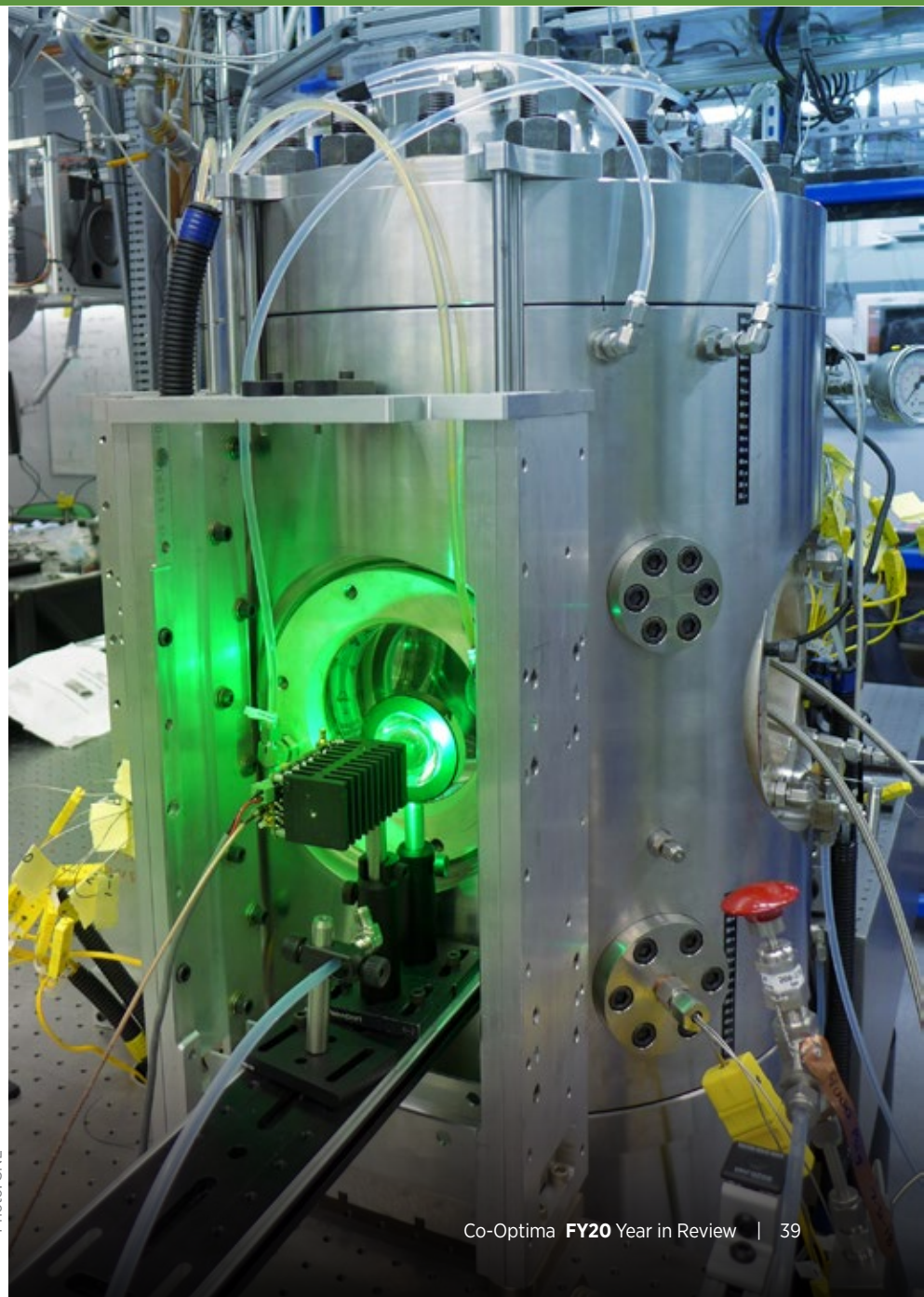


Photo: SNL

NOVEL CATALYSTS AND CONVERSION STRATEGY TURN POLYOXYMETHYLENE ETHERS INTO PROMISING DIESEL BIOBLENDSTOCKS

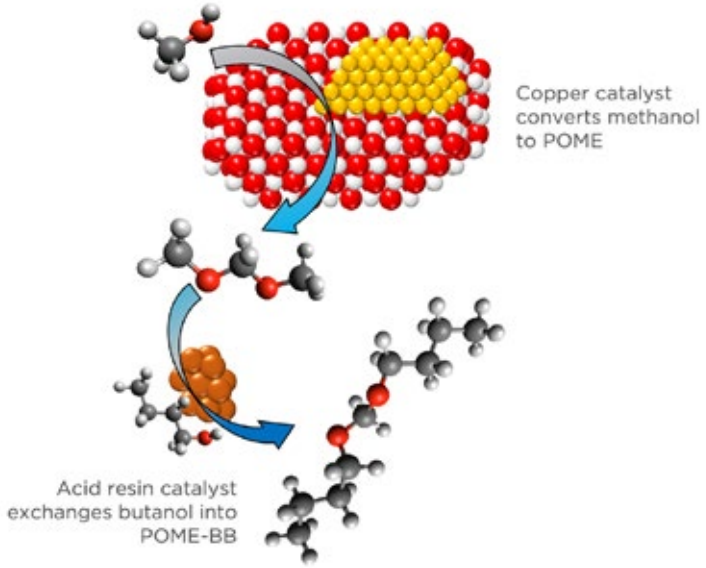
Achievement: Researchers identified a unique POME molecular structure with butyl end groups and developed a novel catalyst and biomass conversion strategy to synthesize this POME-BB structure at high yields.

Potential Impact: Because its energy content is higher and its water solubility lower than the parent POME—and it can be produced under moderate temperatures and pressures—the POME-BB is a potentially high-performance, cost-effective bioblendstock for use in diesel engines.

Co-Optima researchers used a fuel-property-first approach to identify polyoxymethylene dimethyl ether (POME) structure targets that would provide desirable diesel fuel properties, including low water solubility, which is necessary to prevent groundwater contamination that currently limits POME. Structures with butyl end groups, termed POME-BB, offered the most promising improvements.

This motivated the researchers to develop a simple new two-step conversion approach using methanol produced from biomass gasification to generate these molecules. A novel copper catalyst was used to convert methanol into a POME intermediate, and then an acid-catalyzed reaction was developed under atmospheric pressure and mild temperature to produce the POME-BBs. Using this conversion approach, researchers produced sufficient quantities of the POME-BB for experimental fuel property testing.

The measured fuel properties confirmed that POME-BB maintained the high cetane value of the parent POME, with a marked increase in lower heating value from 19 to 30 MJ/kg. Importantly, the yield sooting index remained significantly below that of petroleum diesel. The water solubility of POME-BB was decreased to less than 2 g/L, which greatly exceeds the target metric, overcoming a major limitation of the parent POME. Future research will analyze techno-economic, life cycle, and engine combustion factors related to this promising new fuel.



Schematic of the process from methanol to POME and subsequent butanol exchange to give POME-BB. Figure by Daniel Ruddy, NREL

DUCTED FUEL INJECTION AND OXYGENATED BIOFUEL BLENDS OVERCOME DIESEL'S INTRACTABLE SOOT-NO_X TRADE-OFF

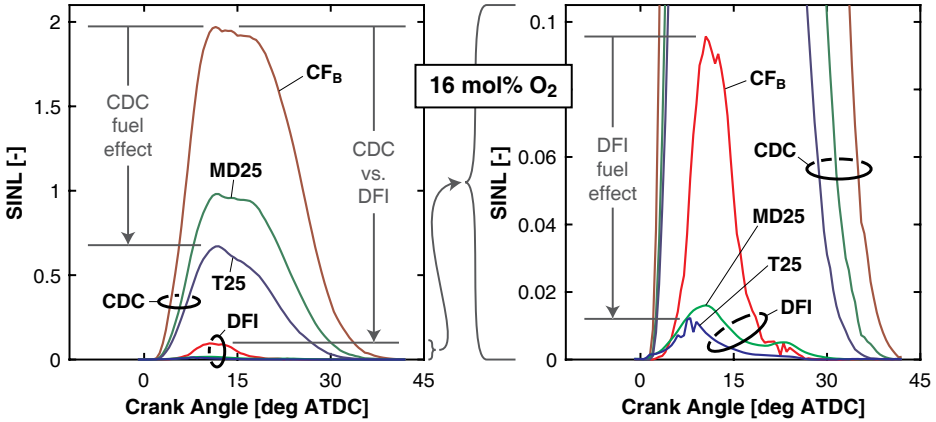
Achievement: At low-NO_X operating conditions, DFI and biofuel blending lowered soot in an MCCI engine by approximately two orders of magnitude relative to conventional diesel combustion of petroleum diesel fuel.

Potential Impact: DFI paired with biofuel blending can break the soot-NO_X trade-off, enabling high-efficiency, cost-effective, clean MCCI engines while adding renewable content to diesel fuels.

MCCI is a highly efficient, time-tested operating strategy for commercial engines, featuring ignition timing that is simple to control. Unfortunately, today's conventional diesel combustion (CDC) approach to MCCI generates problematic levels of soot and NO_X emissions.

Novel Co-Optima-developed DFI technology directs fuel sprays into small ducts aligned with the spray axes in MCCI engines, curbing soot formation by enhancing the level of fuel-air premixing in the autoignition zone. Co-Optima researchers discovered that combining DFI with potential oxygenated biofuels reduces spatially integrated natural luminosity (SINL)—a measure of the amount of hot, in-cylinder soot—by approximately two orders of magnitude relative to CDC of petroleum diesel fuel.

These results were obtained at dilute (low-oxygen) conditions that also reduced NO_X emissions by an order of magnitude relative to undiluted conditions. Although DFI slashes soot and NO_X emissions when petroleum diesel fuel is used, increasing the oxygenated biofuel content reduces emissions further, adds renewable content, and establishes a promising path for the next generation of high-efficiency, cost-effective, high-performance MCCI engines.



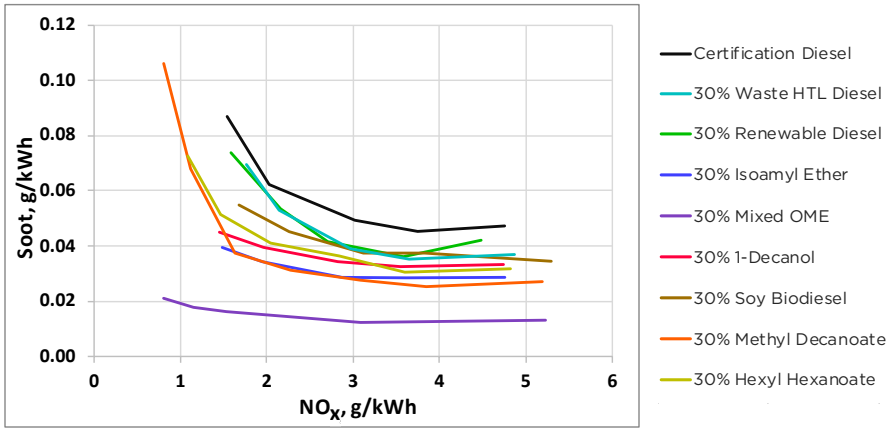
Experimental results comparing in-cylinder levels of hot soot (SINL) for DFI and CDC with three fuels: No. 2 emissions certification diesel (CF_B), 25% blend of methyl decanoate in CF_B (MD25), and 25% blend of tripropylene glycol monomethyl ether in CF_B (T25). Figure shows DFI with each oxygenate blend lowering SINL by approximately two orders of magnitude versus CDC of CF_B. These results are for a 16% intake-oxygen mole fraction, representing an intake dilution level that would be used to control emissions of NO_X. Figure by C.J. Mueller, SNL

BIOMASS-DERIVED BLENDSTOCKS REDUCE MCCI ENGINE NO_X AND SOOT EMISSIONS

Achievement: Researchers quantified the MCCI engine-out NO_X and soot emissions reductions from eight low-net-carbon biofuel blendstocks blended at 30% by volume with conventional diesel fuel.

Potential Impact: Blending low-net-carbon biofuels into diesel for MCCI engines offers the potential for high engine efficiency, fewer harmful tailpipe emissions, and lower life cycle greenhouse gas emissions.

Highly efficient MCCI will likely remain the primary heavy-duty engine technology for decades to come. Co-Optima researchers studied the ability of eight promising biofuel blendstocks identified during Tier 1 screening—two ethers, one alcohol, three esters, and two hydrocarbons—to reduce NO_X and soot emissions when blended at 30% by volume with U.S. Environmental Protection Agency (EPA) emissions certification diesel. Experiments were conducted at three steady-state operating conditions, including the low power level shown in the figure and two higher-power conditions. Relative to the base certification diesel, all of the biofuel blends provided benefits with regard to the soot-NO_X emissions trade-off; increasing levels of exhaust gas recirculation for some of the lowest-sooting fuels reduced NO_X emissions further. Emissions reductions at the low-power condition are particularly important for future emissions compliance because the low exhaust temperatures reduce the effectiveness of emissions controls, in addition to reducing greenhouse gas (GHG) emissions. Ongoing work includes studying how the chemical structure and properties of the blendstocks reduce emissions.



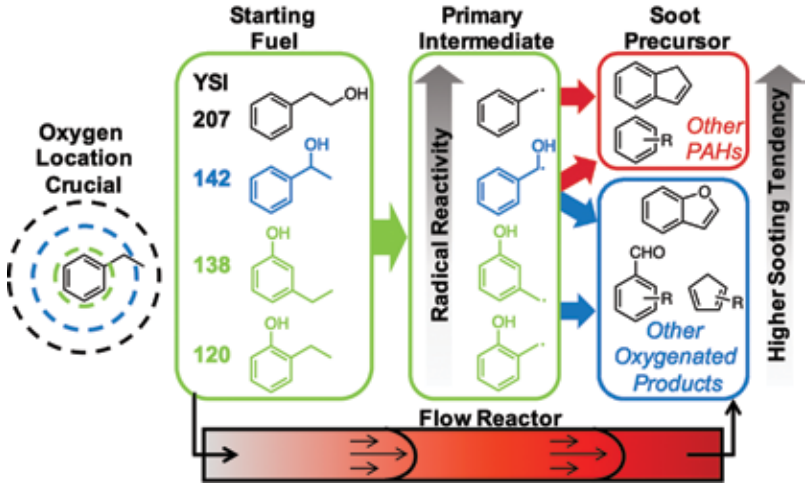
Soot vs. NO_X emissions for EPA emissions certification diesel and eight low-net-carbon biofuel blendstocks blended at 30% by volume with certification diesel, operating at 600 rpm and 3.3-bar gross indicated mean effective pressure (gIMEP), one of the three operating conditions studied. HTL = hydrothermal liquefaction; OME = oxymethylene dimethyl ether. Figure by Jonathan Martin, NREL

OXYGEN LOCATION DICTATES THE SOOTING TENDENCY OF OXYGENATED AROMATICS

Achievement: Researchers showed how chemical structure affects the sooting tendency of oxygenated aromatics.

Potential Impact: This research will aid the design of new oxygenated aromatics with potential to produce fuels that deliver high performance and have low sooting tendencies.

Oxygenated aromatics (OAs) are promising candidates for biofuel blendstocks because they can be readily produced via lignin depolymerization and have higher octane numbers compared to aromatic hydrocarbons and non-aromatic oxygenates. However, for OAs to become environmentally friendly options, they must be designed to have low sooting tendencies. Co-Optima researchers investigated the effects of OA chemical structure on sooting tendency by identifying soot precursors and studying their formation pathways. The researchers performed flow-reactor experiments and quantum-mechanical calculations for four OA compounds: 1-phenylethanol, 2-phenylethanol, 2-ethylphenol, and 3-ethylphenol. The results showed that OA sooting tendency is reduced when the oxygen atom is closer to the aromatic ring. The primary radicals produced during combustion are stabilized by aromatic resonance and oxygen's electronegativity, resulting in less soot formation. This research facilitates the design of low-emission, high-performance oxygenated biofuel blendstocks.



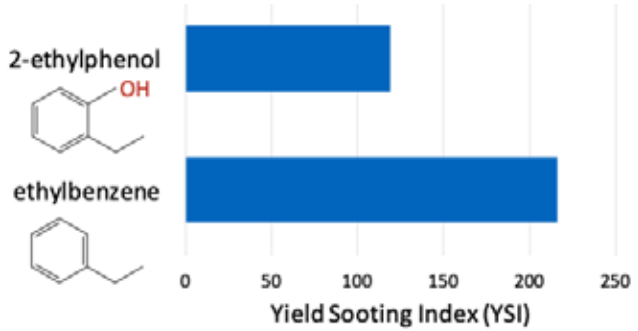
Schematic of how oxygen location affects the primary radical intermediates and their reactivities, resulting in different OA sooting tendencies. The radical intermediates and soot precursors were determined by flow-reactor experiments and quantum-mechanical calculations. PAH = polycyclic aromatic hydrocarbon; YSI = yield sooting index. Figure by Brian Etz, Yeonjoon Kim, and Seonah Kim, NREL

PHENOLIC GROUPS SUPPRESS SOOT PRODUCTION FROM AROMATIC HYDROCARBONS

Achievement: Experiments demonstrated that phenolic groups suppress soot formation from aromatic hydrocarbons, and theoretical calculations identified the chemical mechanisms that cause this suppression.

Potential Impact: This fundamental knowledge provides a basis for identifying lignin-derived bioblendstocks that offer the fuel property benefits of aromatic hydrocarbons without the high soot emissions.

Aromatic hydrocarbons offer many useful fuel properties, such as high energy density, but they tend to form high concentrations of carbon soot particles during combustion. Co-Optima researchers performed experiments demonstrating that the addition of phenolic functional groups to aromatic molecules can suppress this soot formation. For example, the phenol-substituted ethylbenzene compound 2-ethylphenol produced 45% less soot than ethylbenzene alone when burned in a standardized laboratory flame. The researchers used quantum chemistry calculations, molecular dynamics simulations, and detailed flame modeling to analyze the experimental measurements and identify the chemical mechanisms underlying this soot suppression. Both alkylbenzenes and alkylphenols react to form resonance-stabilized radicals by cleavage of the weakest bond. Radicals formed from alkylbenzenes such as ethylphenol have a low energy barrier for coupling to form polyaromatic hydrocarbons, which are well-known soot precursors. Oxygenated radicals formed from alkylphenols react to form oxygenated aromatics such as benzaldehydes or benzofurans with much lower sooting tendency. Although chemical compounds containing phenolic groups do not occur in petroleum, they are abundant in the lignin portion of biomass. The results of this study provide the fundamental knowledge necessary to identify phenolic bioblendstocks that can be produced economically and sustainably from lignin and can offer the benefits of aromatic hydrocarbons without the high soot emissions.



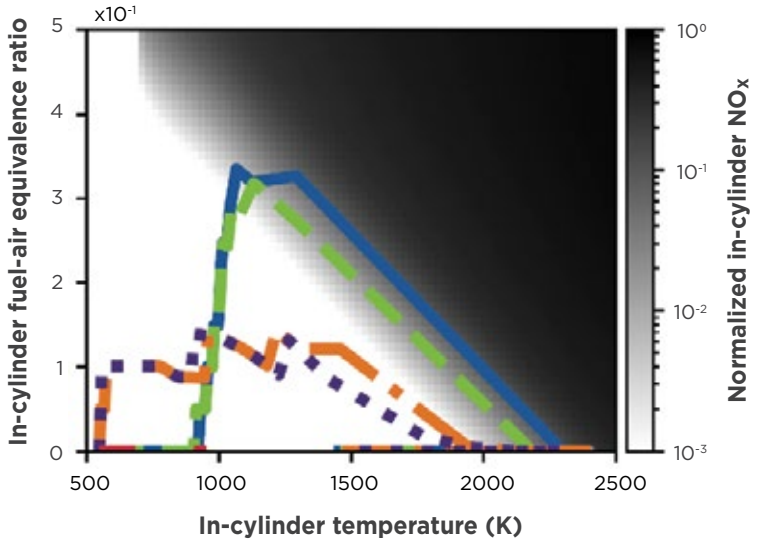
Experimental yield sooting index results showing that 2-ethylphenol, a phenol-substituted compound from the aromatic hydrocarbon ethylbenzene, produces 45% less soot than ethylbenzene itself. Figure by Charles McEnally, Yale University

DEEP REINFORCEMENT LEARNING SHOWS POTENTIAL TO OPTIMIZE WORK AND EMISSIONS IN COMPRESSION-IGNITION ENGINES

Achievement: Deep reinforcement learning was used to find new CI injection strategies that reduce NOx emissions while maintaining work output.

Potential Impact: Optimizing work and emissions through deep reinforcement learning could facilitate development of clean and efficient CI engines.

One popular strategy for reducing emissions from compression-ignition (CI) engines is to split the fuel injection into a series of smaller injections. Co-Optima researchers explored the use of deep reinforcement learning (DRL) to discover optimal CI engine control strategies. A DRL agent learns autonomically by receiving a "reward" signal after interacting with an environment. In this case, a DRL agent was trained to maximize work while minimizing in-cylinder NO_x production in a CI engine model. When the priority for work was high, the agent learned to inject near top dead center to maximize total work, generating large amounts of NO_x. When the priority for work was low, the agent learned to tailor its injection schedule to operate in the low-temperature combustion (LTC) regime, reducing NO_x production. Using a simplified engine model, the DRL agent reduced NO_x emissions threefold while decreasing net work by only 2%. This technique is currently being adapted to control in-cylinder fuel blending to co-optimize fuels with a specific engine design.



Equivalence ratio vs. temperature pathways for five different injection schedules discovered by the DRL agent. As the priority shifts toward reducing NO_x emissions—that is, as the injection schedules shift from blue (highest NO_x emissions) to green, orange, purple, and then red (lowest NO_x emissions)—the injection schedule operates increasingly in the LTC region to reduce in-cylinder NO_x production. Figure by Nicholas Wimer, NREL

MCCI FUELS FROM WASTE FEEDSTOCKS SHOW LOW GHG EMISSIONS

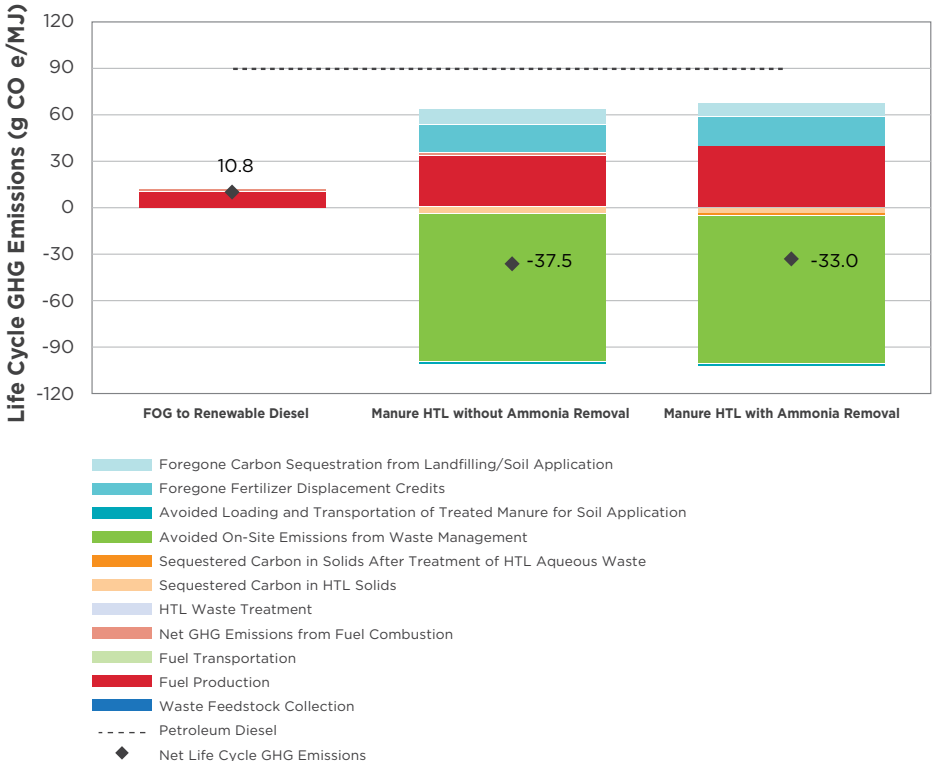
Achievement: LCA results showed that MCCI bioblendstocks produced from FOG and swine manure can result in GHG reductions of 87% to more than 100% relative to petroleum diesel.

Potential Impact: These waste feedstocks offer additional opportunities to produce cost-effective, energy-efficient, and low-emission MCCI bioblendstocks with the potential for accelerated production ramp-up via mature or pilot-stage pathways.

Co-Optima researchers developed detailed process models to evaluate the economic, energy, and environmental attributes of MCCI bioblendstocks produced via two pathways: hydrothermal liquefaction (HTL) of swine manure and hydroprocessing of used cooking oil and brown grease (grease collected in traps to prevent clogging sewers). These feedstocks are concentrated forms of biomass available at low prices—or even negative prices, because their producers may pay to have them removed to avoid waste-management costs.

The swine manure HTL pathway features a decoupled upgrading plant design to reduce cost through economies of scale, offering greater biocrude and MCCI fuel yields and high-quality MCCI fuel with a high cetane number (about 70). Life cycle analysis (LCA) results showed that swine manure to MCCI diesel via HTL could reduce GHG emissions by more than 100%, via avoidance of methane emissions that could occur from waste manure management practices. Sensitivity analysis revealed that scaling up the HTL plant from 110 to 250 short tons per day can increase the swine manure HTL yield to 85% and improve the catalyst lifetime.

The relatively mature fats, oils, and greases (FOG) pathway inherently has higher product yields compared to other biochemical conversion technologies for lignocellulosic feedstocks, producing high-quality MCCI fuel with a high cetane number and low levels of aromatics and sulfur, although availability of waste grease resources poses a constraint. MCCI bioblendstocks produced from FOG via hydroprocessing reduce GHG emissions by about 87%. Continued development of waste conversion pathways in conjunction with analysis of environmental benefits should help realize the potential benefits identified in this analysis.



Life cycle GHG emissions results for MCCI bioblendstocks produced with FOG via hydroprocessing and swine manure via HTL. Figure by Ling Tao (NREL), Shuyun Li (PNNL), Longwen Ou (ANL), and Hao Cai (ANL)

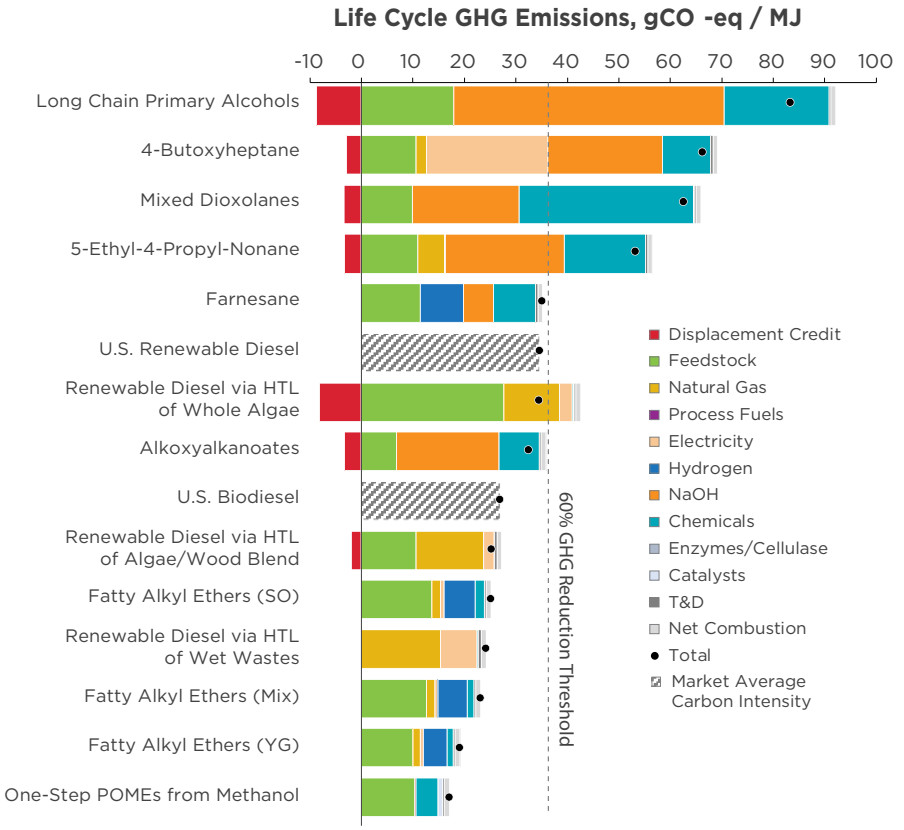
ANALYSIS REVEALS FIVE PROMISING MCCI BIOBLENDSTOCKS THAT CAN REDUCE MD AND HD GHG EMISSIONS BY UP TO 81%

Achievement: Life cycle GHG results for nine bioblendstocks indicate five blendstocks, in addition to two market MCCI bioblendstocks, can reduce GHG emissions by at least 60%.

Potential Impact: Production and use of these blendstocks can help reduce GHG emissions relative to that produced by petroleum diesel fuel used for MD and HD ground transportation.

Co-Optima researchers assessed the life cycle GHG emissions of 13 pathways for producing nine bioblendstocks with properties favorable for co-optimization with MCCI engines. Two blendstocks already on the market (U.S. Renewable Diesel and U.S. Biodiesel) were compared to nine additional candidates derived from biomass, algae, and wet wastes. This assessment, especially at early stages of research, provides a natural feedback loop to inform process design and guide the development of sustainable fuels. The life cycle GHG emissions were evaluated using Argonne National Laboratory's 2020 GREET (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) model.

Life cycle GHG emissions ranged from 17 to 83 g of CO_2 equivalent per megajoule (gCO_2e/MJ) across the bioblendstocks, with the sources of GHG emissions varying substantially. Overall, the analysis showed feedstocks, electricity, natural gas, hydrogen, sodium hydroxide, and other chemical inputs as the primary contributors to GHG emissions. Of the nine bioblendstocks examined, five blendstocks—farnesane, renewable diesel from algae and wet wastes, alkoxyalkanoates, fatty alkyl ethers, and one-step POMEs—produced via nine pathways showed potential to reduce GHG emissions 61%–81% relative to a baseline petroleum diesel fuel. These results show that a variety of feedstocks and production pathways can be used to generate blendstocks that meet fuel property and life cycle GHG emissions targets.



Life cycle GHG emissions for MCCI blendstock candidates by GHG source. Red bars reflect credits associated with displacing emissions for co-products of bioblendstock production. Black dots denote net GHG emissions. SO = soybean oil, YG = yellow grease, Mix = 60:40 mix of SO and YG. Figure by Greg Zaimes with contributions from Longwen Ou, P. Thathiana Benavides, and Troy Hawkins, ANL

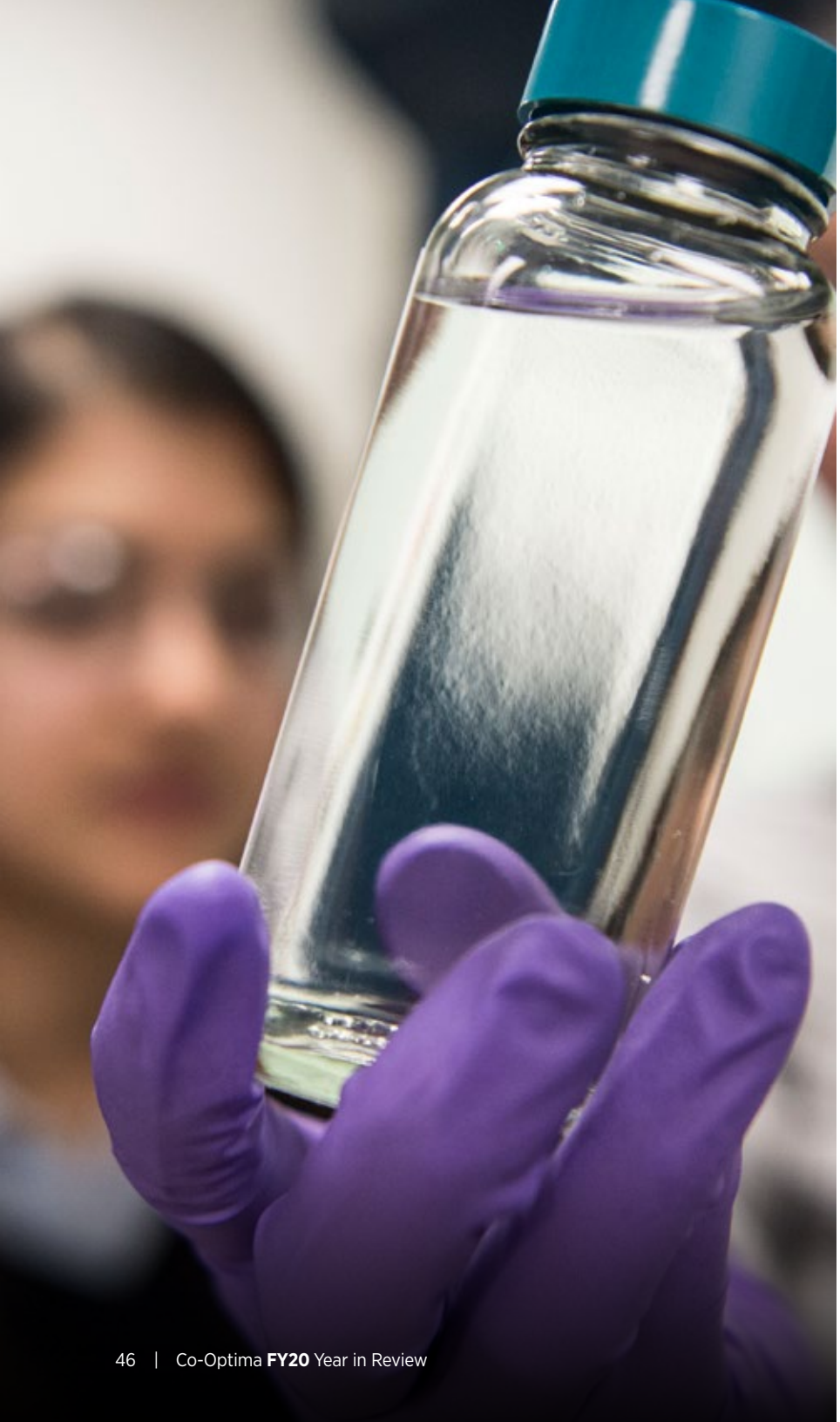


Photo: NREL

EXPANDED SCREENING IDENTIFIES DIESEL-RANGE MCCI BIOBLENDSTOCK CANDIDATES WITH POTENTIAL FOR SUSTAINABILITY AND COMMERCIALIZATION

Achievement: Researchers assessed 14 MCCI bioblendstocks for technological readiness, economic viability, and environmental impact using techno-economic and life cycle analyses.

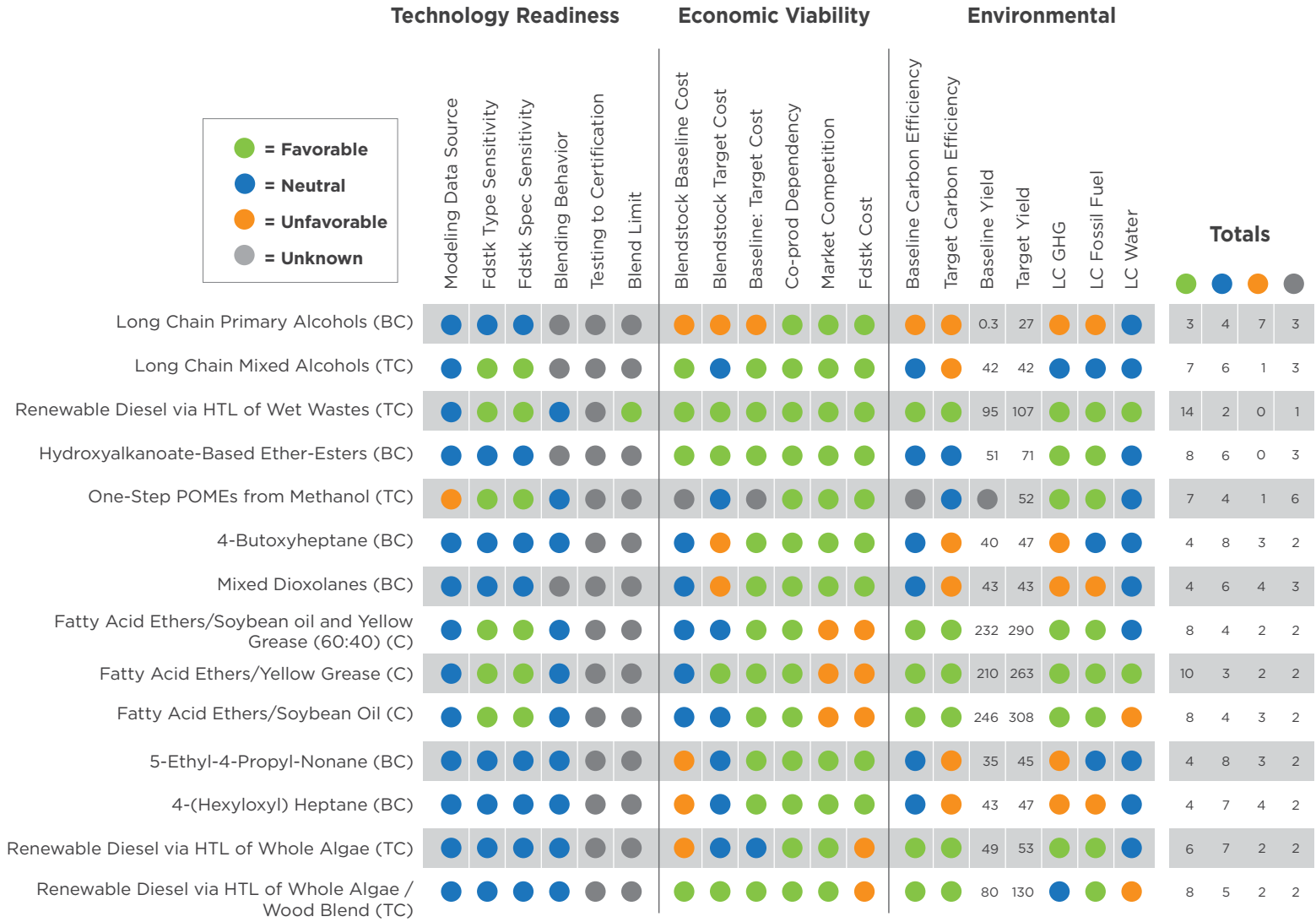
Potential Impact: These analyses help gauge prospects for reducing the GHG emissions of MD and HD transportation at a commercial scale while focusing fuels research and development (R&D) on improvements that provide the greatest performance benefits.

Over the last two years, Co-Optima researchers assessed the sustainability and commercialization potential of 14 bioblendstocks for use with diesel in MCCI engines. Techno-economic and life cycle analyses were used to assess and rank candidate fuels against 19 metrics for technology readiness, economic viability, and environmental impacts. Most candidate blendstocks offered favorable economic metrics, four with target case prices below $4/GGE. The target cases reflect improved process performance, anticipated to be achieved with further research.

Conversion of residual lignin from corn stover to valuable coproducts for biochemical pathways could further reduce target selling prices. Seven blendstocks showed potential to reduce both GHG emissions and fossil energy consumption by 60%–80% compared with conventional diesel fuel. Renewable diesel produced via HTL of wet wastes and fatty acid ethers produced from used cooking oil (yellow grease) delivered the most favorable metrics of the bioblendstocks evaluated, demonstrating strong economic potential and significant reductions in environmental impact.

Industrial-scale production of these fuels faces challenges with limited availability of used cooking oil and wet waste feedstocks such as livestock manure and wastewater treatment residuals. The biomass-conversion technologies for most candidate blendstocks are robust, experiencing little impact from variations in biomass feedstock type and quality. Many of these diesel bioblendstocks are at a lower technological readiness level compared with more mature gasoline bioblendstocks.

Co-Optima continues to build understanding of technology readiness, blending behavior, and legal limits on blend levels by screening potential MCCI bioblendstocks across a wide spectrum of chemical structures, feedstock types, and conversion technologies. Research and analysis are still needed to advance conversion technologies to make these blendstocks, along with a better understanding of impacts on engine performance.



Techno-economic and life cycle analysis results for the 14 evaluated Co-Optima MCCI bioblendstock pathways. Results are categorized and compared based on favorability for each metric. Production routes generally do not include coproducts. Favorable, neutral, and unfavorable thresholds for each category were set in consultation with conversion and fuel experts. Life cycle GHG, fossil, and water metrics, as well as feedstock cost, represent a future target case. Baseline and target yields are expressed in GGE per dry U.S. ton. BC = biochemical, C = catalytic, Fdstk = feedstock, LC = life cycle, spec = specification, TC = thermochemical. Figure by Andrew Bartling (NREL) and P. Thathiana Benavides (ANL), with contributions from Steven Phillips (PNNL), Troy Hawkins (ANL), and Avantika Singh (NREL)

SULFUR REDUCTION AND CETANE IMPROVEMENT FROM MCCI BIOBLENDSTOCKS OFFER VALUE TO PETROLEUM REFINERS

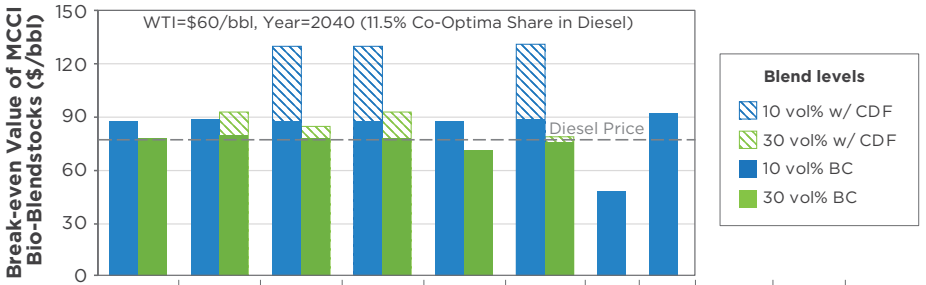
Achievement: A refinery impact analysis showed that low sulfur content can increase the breakeven value of diesel-range bioblendstocks to petroleum refiners, and bioblendstocks with high cetane numbers could create extra value in a market that has demand for high-cetane diesel.

Potential Impact: The results suggest potential market opportunities for diesel-range bioblendstocks in the petroleum industry, in alignment with industry-standard methods for maximizing economic benefits.

Bioblendstocks may help petroleum refiners adapt to evolving market demands for fuels with better properties that meet increasingly stringent regulations. Co-Optima researchers analyzed the breakeven value to refiners of eight diesel-boiling-range MCCI bioblendstock candidates that have high cetane numbers and low sulfur contents. The breakeven value is the maximum purchase cost for a bioblendstock that maintains the profitability associated with a petroleum-based fuel that refiners would otherwise use.

The analysis was performed using full refinery linear programming models based on representative refinery configurations from the U.S. Energy Information Administration (EIA), blending properties of MCCI bioblendstocks from Co-Optima measurements, ASTM fuel specifications, price data from the Oil Price Information Service, and future fuel market projections from EIA and the National Renewable Energy Laboratory's Automotive Deployment Options Projection Tool (ADOPT). The bioblendstocks were evaluated at 10% and 30% blends (by volume) in two cases. In the base case, only ultra-low sulfur diesel (ULSD) was prevalent in the market. In the alternative case, the diesel market was served by both ULSD and the high-cetane California diesel fuel (CDF).

The results indicated that a bioblendstock with an extremely low sulfur content and a very high cetane number may offer refiners a breakeven value 1.5 times as high as the price of petroleum-based diesel in a future fuel market. Sulfur content had the most significant impact on value, while high cetane number created extra value in the alternative case owing to that case's demand for high-cetane diesel.



Properties	2-Nonanol	Methyl decanoate	Dipentyl ether	4-butoxy heptane	5-ethyl-4-propyl-nonane	Soy biodiesel	HTL diesel	OMEs	Petro-diesel	ULSD Specs	CDF Specs
Cetane number	38-41	46-52	91-96	57-65	48	54-55	65.8	93	50	>40	>53
Specific gravity	0.827	0.873	0.783	0.802	0.763	0.888	0.813	1.109	0.816	<0.876	<0.84
Sulfur, ppmw	0	0	0	0	0	0	-56	0	15	<15	<15

Breakeven values of diesel-range bioblendstocks to petroleum refiners—solid bars for the base case (ULSD only), striped bars for the alternative case (ULSD + CDF)—showing correlations between values and fuel properties. Some properties are color-coded: red means off-specification, orange means meets criterion, blue means exceeds criterion, and green means greatly exceeds criterion. The sulfur content of diesel from HTL depends on the feedstocks used to produce it, and it may be reduced via ongoing R&D. bbl = barrel; BC = base case; OMEs = oxymethylene ethers; ppmw = parts per million weight; WTI = West Texas Intermediate. Figure by Yuan Jiang, PNNL

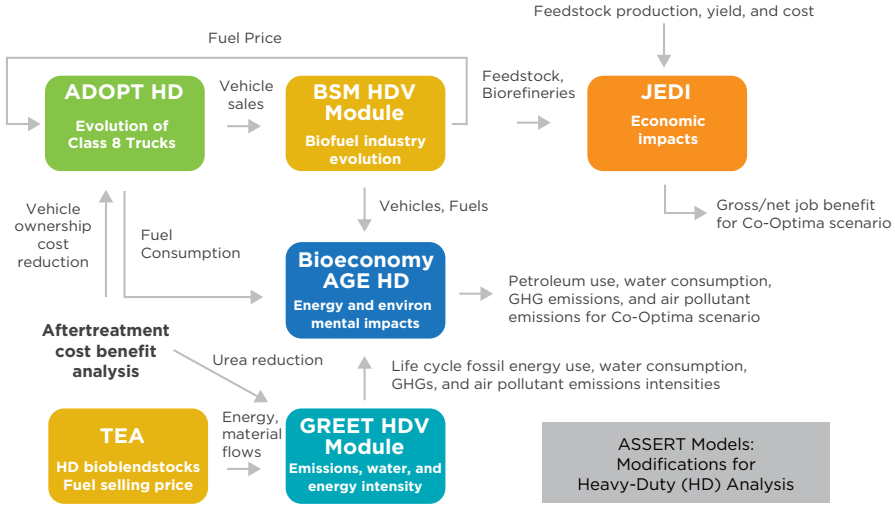
NEW MODELING CAPABILITIES EXPLORE EMISSIONS BENEFITS OF CO-OPTIMIZED HEAVY-DUTY MCCI FUELS AND ENGINES

Achievement: Modeling capabilities were enhanced to enable simulation of Co-Optima HD technology deployment, and a preliminary analysis examined the potential benefits of deploying Class 8 trucks using a 10% biofuel blend.

Potential Impact: These integrated models provide an important tool set for assessing the potential environmental benefits of adopting Co-Optima HD technologies.

Researchers developed Co-Optima modeling capabilities to simulate the benefits of deploying HD MCCI fuel and engine technologies. This included enhancements to ADOPT; the Biomass Scenario Model (BSM); and the Bioeconomy Air emissions, Greenhouse gas emissions, and Energy consumption (Bioeconomy AGE) model. The researchers used the new capabilities to analyze the potential benefits of co-optimized Class 8 trucks fueled with a 10% biofuel blend. They conservatively assumed that co-optimization of MCCI engines with this biofuel blend saves $600 in aftertreatment costs over the lifetime of a Class 8 vehicle, based on reducing engine-out NO_x and PM emissions by 10%.

Preliminary results projected significant purchases of these vehicles in the United States, reducing cumulative GHG emissions by 7.5% between 2025 and 2050 relative to a business-as-usual scenario. These findings suggest that development and scale-up of co-optimized MCCI technology and biofuel blends for HD vehicles could lead to meaningful benefits for consumers and the environment.



Integrated modeling for economic and environmental benefit analysis of large-scale deployment of co-optimized fuel and engine technologies, highlighting model enhancements for HD applications. GREET = Greenhouse gases, Regulated Emissions, and Energy use in Technologies; HDV = heavy-duty vehicle; JEDI = Jobs and Economic Development Impact. Figure by Jennifer Dunn, Hao Cai, and Greg Zaimes (ANL) and Emily Newes (NREL)

NEXT STEPS

In the coming year, the Co-Optima initiative will shift even more strongly toward medium-duty (MD) and heavy-duty (HD) advanced compression-ignition (ACI) and multimode approaches that also include mixing-controlled compression ignition (MCCI) engine and fuels research. The MD/HD research portfolio includes blendstocks and fuels in both the diesel and gasoline volatility ranges.

The gasoline-range research will leverage earlier Co-Optima light-duty (LD) multimode studies to improve the team's understanding of fuel properties, autoignition, and ACI combustion. Additional MD/HD research will focus on analyses based on previous years' findings.

In Fiscal Year 2021 (FY21), the Co-Optima team plans to pursue the following goals:

LD Multimode

- Develop a fuel property metric to capture fuel autoignition behavior for spark-ignition (SI)/ACI engines
- Assess fuel property impacts on engine efficiency, fuel economy, and emissions
- Conduct additional analyses for candidate blendstocks, including refinery impacts and the potential for impact at scale
- Identify emissions compliance strategies for a multimode SI/ACI engine.

MD/HD MCCI

- Conduct techno-economic, life cycle, and refinery benefits analyses for candidate blendstocks, including the potential for impact at scale
- Determine if development of multimode or hybrid electrification technologies for diesel vehicles can provide additional benefits, assess potential fuel savings, and conduct analyses of other techno-economic and life cycle factors.

MD/HD ACI

- Demonstrate high-performance blendstocks' potential to enhance combustion-phasing control in MD/HD ACI engines while maintaining low emissions
- Determine the potential for diesel-range fuel properties to enable low-load ACI operation in MD/HD engines with ultra-low emissions and low exhaust temperatures
- Identify blendstocks that provide key fuel properties.

Co-Optima is also developing plans to share the significant body of knowledge discovered through the work of this initiative, in order to deliver the objective scientific basis necessary for American industry leaders and policymakers to formulate informed decisions. Plans under discussion include but are not limited to webinars, capstone publications, and one-on-one stakeholder engagement.

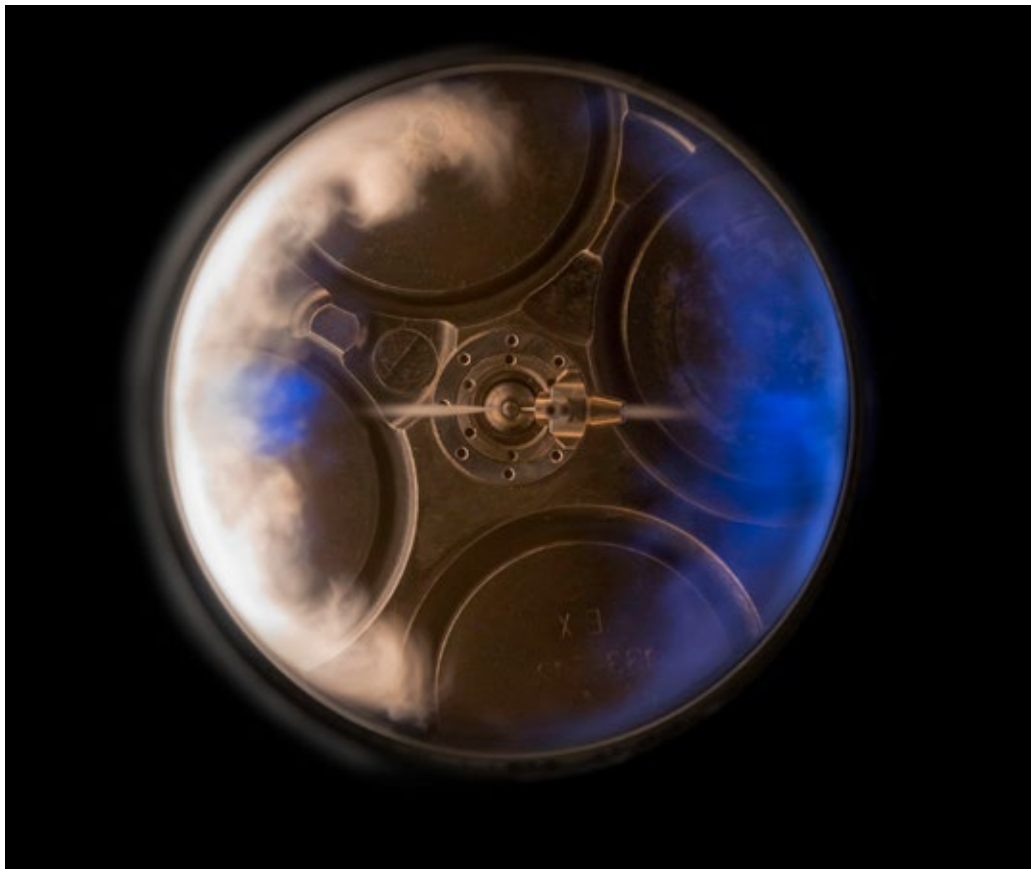


Photo: SNL

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.

A machine-Learning derived, Fast, Accurate Bond dissociation Enthalpy Tool (ALFABET)
https://bde.ml.nrel.gov/
ALFABET makes it possible for researchers to identify the most promising fuels for lower emissions and greater engine efficiency in seconds rather than days. Using ALFABET to determine bond dissociation enthalpy (BDE)—the energy required to break a chemical bond between atoms in organic compounds—allows researchers to predict chemical reactions and determine suitability for certain uses, including biofuels.

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 trade-offs 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 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 yield sooting index (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.

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 1,000 biobased fuel blendstocks, as well as 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 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.

PUBLICATIONS AND MEDIA COVERAGE

Co-Optima researchers have continued their strong scientific publication track record, with more than 60 journal articles, conference papers, technical reports, and other research publications issued during Fiscal Year 2020 (FY20). These publications span light-duty (LD), medium-duty (MD), and heavy-duty (HD) applications, blendstock structure-property relationships, emissions, new analytical tools, and techno-economic and life cycle analyses. The Co-Optima publications database (https://www.energy.gov/eere/bioenergy/co-optima-publications-library-0) now totals more than 240 entries. Beyond the publications developed by Co-Optima participants, various Co-Optima activities were covered by trade and popular media outlets in FY20.

HIGH-IMPACT PUBLICATIONS

Four FY20 articles published in particularly high-impact journals are highlighted below, illustrating both the culmination of long-running Co-Optima research and development (R&D), as well as ongoing work. Publication in such journals confirms the significance and credibility of Co-Optima findings while disseminating findings to key audiences.

"What fuel properties enable higher thermal efficiency in spark-ignited engines?"
Progress in Energy and Combustion Science [Vol. 82, September 2020 (online)]
Authors: J.P. Szybist, S. Busch, R.L. McCormick, J.A. Pihl, D.A. Splitter, M.A. Ratcliff, C.P. Kolodziej, J.E. Storey, M. Moses-DeBusk, D. Vuilleumier, M. Sjöberg, C.S. Sluder, T. Rockstroh, and P. Miles
https://doi.org/10.1016/j.pecs.2020.100876

- Co-Optima research demonstrated how the effects of six fuel properties—research octane number, octane sensitivity, latent heat of vaporization, laminar flame speed, particulate matter index, and catalyst light-off temperature—can be combined into a unified merit function and used to assess the potential of bioblendstocks to enable high thermal efficiency in boosted spark-ignition (SI) engines for LD vehicles.
- This article shares scientific details on the initiative's research on turbocharged SI engines that will help the research community and industry identify viable candidates for high-performance biobased fuels.

"Energy, economic, and environmental benefits assessment of co-optimized engines and bio-blendstocks"
Energy & Environmental Science [Issue 8, June 2020]
Authors: J.B. Dunn, E. Newes, H. Cai, Y. Zhang, A. Brooker, L. Ou, N. Mundt, A. Bhatt, S. Peterson, and M. Biddy
https://doi.org/10.1039/D0EE00716A

- Researchers modeled deployment of LD engines co-optimized with three biofuel blends to deliver 10% higher engine efficiency, quantifying potential effects on U.S. petroleum consumption, greenhouse gas emissions, particulate matter emissions, water consumption, and jobs.
- The analysis described in this article provides a framework for evaluating the energy, environmental, and economic benefits of deploying co-optimized fuels and engines.

"Performance-advantaged ether diesel bioblendstock production by a priori design"
Proceedings of the National Academy of Sciences [Vol. 116, No. 52, December 2019]
Authors: N.A. Huq, X. Huo, G.R. Hafenstine, S.M. Tifft, J. Stunkel, E.D. Christensen, G.M. Fioroni, L. Fouts, R.L. McCormick, P.A. Cherry, C.S. McEnally, L.D. Pfefferle, M.R. Wiatrowski, P.T. Benavides, M.J. Biddy, R.M. Connatser, M.D. Kass, T.L. Alleman, P. St. John, S. Kim, and D.R. Vardon
https://doi.org/10.1073/pnas.1911107116

- Researchers examined fuel properties and pathways to production optimization for the oxygenated biofuel 4-butoxyheptane, identifying its potential to improve ignition quality, reduce soot and greenhouse gas emissions, achieve economic competitiveness, and maintain compatibility with fueling infrastructure when blended with petroleum-based diesel.

- The article outlines an approach to developing market-ready biofuels for MD and HD vehicles that accounts for performance, environmental impact, infrastructure compatibility, and economic feasibility.

"Prediction of organic homolytic bond dissociation enthalpies at near chemical accuracy with sub-second computational cost"
Nature Communications [Vol. 11, May 2020]
Authors: P.C. St. John, Y. Guan, Y. Kim, S. Kim, and R.S. Paton
https://doi.org/10.1038/s41467-020-16201-z

- A machine-learning method for predicting organic molecule bond dissociation enthalpy (the energy required to break bonds between atoms and a key driver of chemical reactions) demonstrated prediction speeds of less than a second and accuracy rivaling the uncertainty associated with experimental measurements.

- The method outlined in the article—and recently made available in the online A machine-Learning derived, Fast, Accurate Bond dissociation Enthalpy Tool (ALFABET)—breaks the traditional trade-off between predictive accuracy and computational cost, helping researchers identify potentially low-emission, high-efficiency biofuel molecules in seconds rather than days.

For more detailed information on other Co-Optima publications, see the following pages and the online database:
https://www.energy.gov/eere/bioenergy/co-optima-publications

Selected Publications and Notable Presentations

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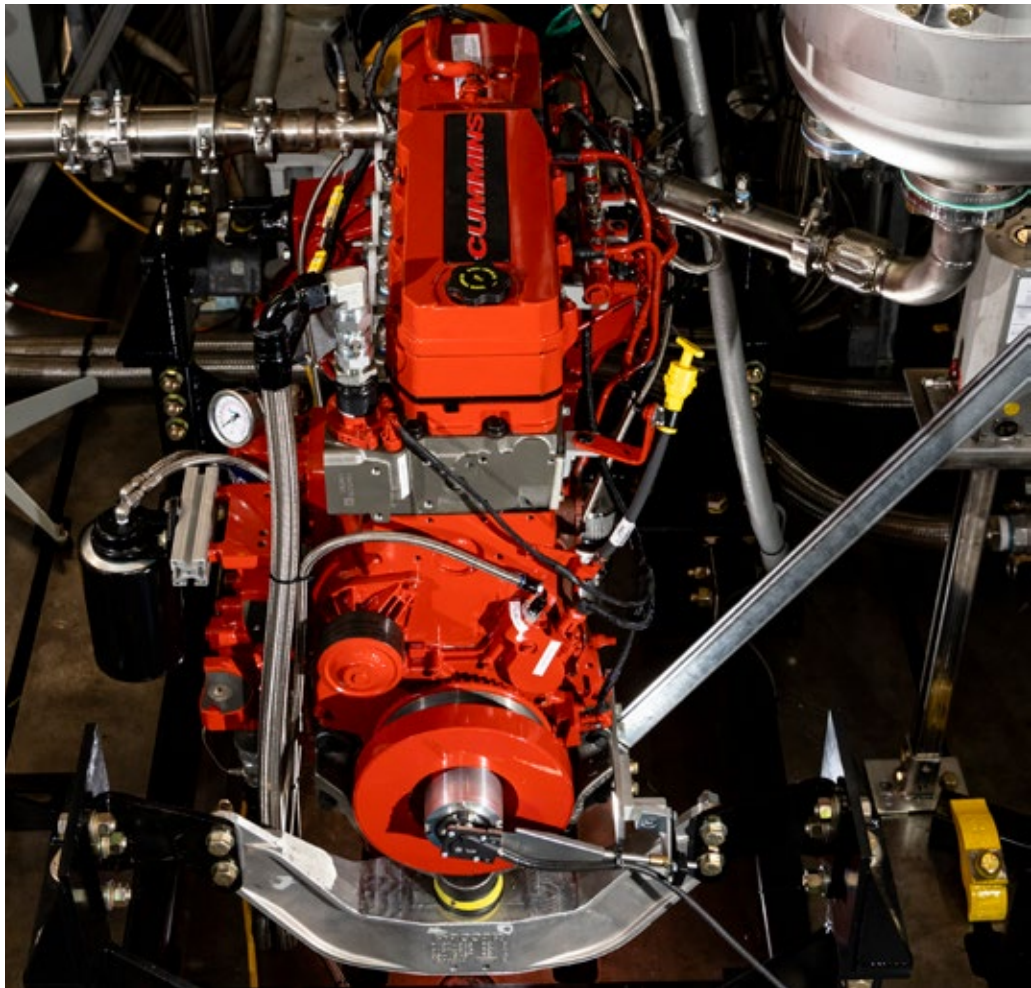

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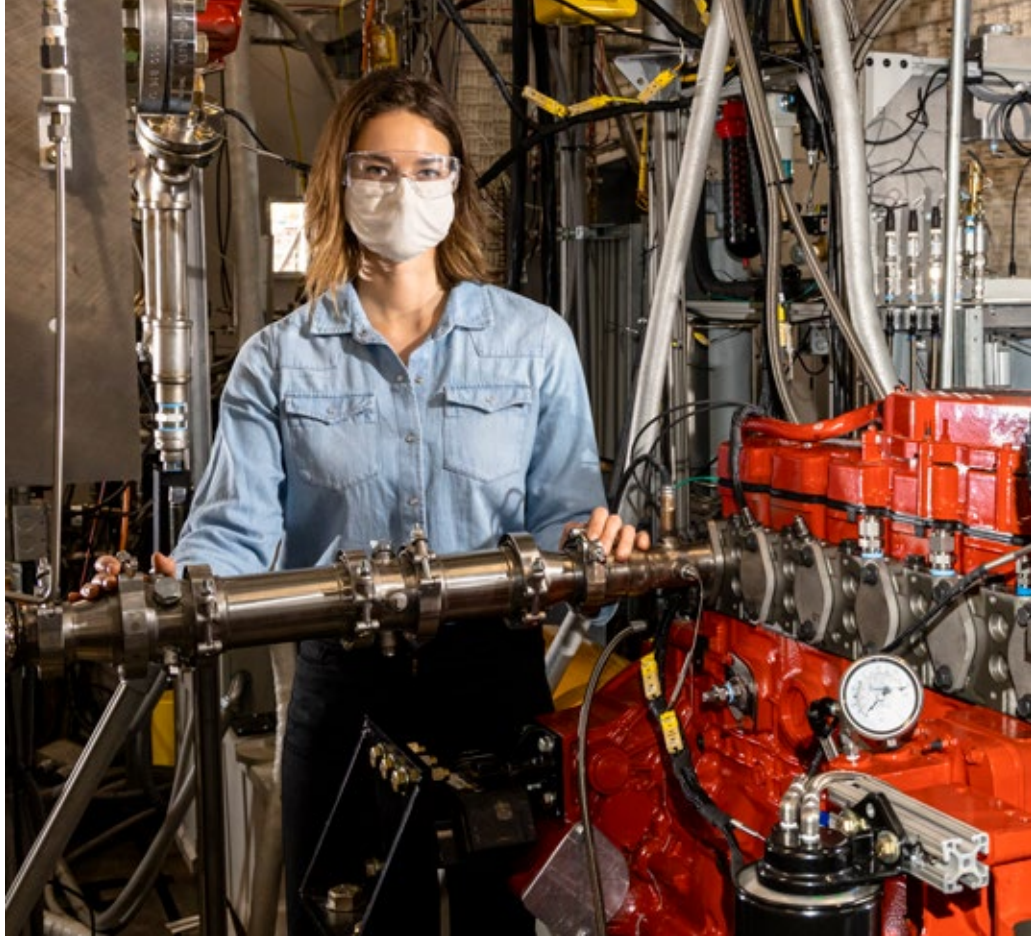


Photos: ORNL, PNNL (top to bottom)

ACRONYMS AND ABBREVIATIONS

^{1}H NMR .....proton nuclear magnetic resonance

ABLC .....Advanced Bioeconomy Leadership Conference

ACI .....advanced compression ignition

ADOPT.....Automotive Deployment Options Projection Tool

AHRR .....apparent heat-release rate

ALFABET .....A machine-Learning derived, Fast, Accurate Bond dissociation Enthalpy Tool

ANL .....Argonne National Laboratory

ATDC .....after top dead center

bbl .....barrel

BDE .....bond dissociation enthalpy

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

BMEP .....brake mean effective pressure

BMON .....beyond motor octane number

BOB .....blendstock for oxygenate blending

BRON .....beyond research octane number

bTDC .....before top dead center

CA10 .....crank angle at which 10% of the fuel has burned

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

CAD .....crank angle degree

CDC .....conventional diesel combustion

CDF .....California diesel fuel

CFD .....computational fluid dynamics

CFR .....Cooperative Fuel Research

CI .....compression ignition

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

DC3 .....direct catalytic conversion of cellulosics

DFI .....ducted fuel injection

DFO .....Directed Funding Opportunity

DFT .....density functional theory

DMF .....dimethylfuran

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

DRL .....deep reinforcement learning

E10 .....gasoline containing 10% ethanol

E30 .....gasoline containing 30% ethanol

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

EGR .....exhaust gas recirculation

EIA .....U.S. Energy Information Agency

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

FOG .....fats, oils, and greases

FY .....fiscal year

GGE .....gasoline gallon equivalent

GHG .....greenhouse gas

GP .....Gaussian process

HC .....hydrocarbon

HCCI .....homogeneous-charge compression ignition

HD .....heavy duty

HOV .....heat of vaporization

HPC .....high-performance computing

HTL .....hydrothermal liquefaction

ITHR .....intermediate-temperature heat release

LANL .....Los Alamos National Laboratory

LBNL .....Lawrence Berkeley National Laboratory

LCA .....life cycle analysis

LD .....light duty

LHV .....lower heating value

LLNL .....Lawrence Livermore National Laboratory

LSPI .....low-speed pre-ignition

LTC .....low-temperature combustion

LTGC .....low-temperature gasoline combustion

LTHR .....low-temperature heat release

MCCI .....mixing-controlled compression ignition

MD .....medium duty

MON .....motor octane number

NO_x .....nitrogen oxides

NREL .....National Renewable Energy Laboratory

OA .....oxygenated aromatic

ORNL .....Oak Ridge National Laboratory

PFS .....partial fuel stratification

PM .....particulate matter

PMI .....particulate matter index

PNNL .....Pacific Northwest National Laboratory

POME .....polyoxymethylene dimethyl ether

POME-BB .....polyoxymethylene dimethyl ether with butyl end groups

ppm .....parts per million

PRF .....primary reference fuel

PSHR .....pre-spark heat release

R&D .....research and development

RBOB .....reformulated blendstock for oxygenate blending

RCM .....rapid-compression machine

RMG .....Reaction Mechanism Generator

RON .....research octane number

RVP .....Reid vapor pressure

S .....octane sensitivity

SACI .....spark-assisted compression ignition

SI .....spark ignition

SINL .....spatially integrated natural luminosity

SNL .....Sandia National Laboratories

SOI .....start of injection

TDC .....top dead center

TEA .....techno-economic analysis

TSF .....toluene standardization fuel

TWC .....three-way catalyst

ULSD .....ultra-low-sulfur diesel

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

YSI .....yield sooting index

Zero-RK .....Zero-order Reaction Kinetics

Photos: NREL, ORNL, LBNL (top to bottom)

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 an emissions control catalyst starts to eliminate pollutants

cetane number ..... Measure of the ignition quality of diesel fuel; the higher this number, the more rapidly the fuel ignites after the start of fuel injection in a standard (direct-injection) diesel engine

compression ignition ..... Combustion approach that achieves autoignition through compression of the fuel-air mixture in the cylinder

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

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

ducted fuel injection (DFI) ..... Method for enhancing fuel-air mixing in MCCI engines by directing fuel sprays into small, 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

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

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 autoignition of unburned fuel/air mixture in a spark-ignition engine 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 (a linear blending model)

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 the combustion rate 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 high-intake-temperature 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), interpreted as the temperature sensitivity of autoignition

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 in SI engines

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 or equivalence ratio (phi)

Reid vapor pressure (RVP) ..... Vapor pressure measured at 38°C and an indicator of fuel volatility

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

soot ..... Elemental carbon particles produced in engines from incomplete combustion

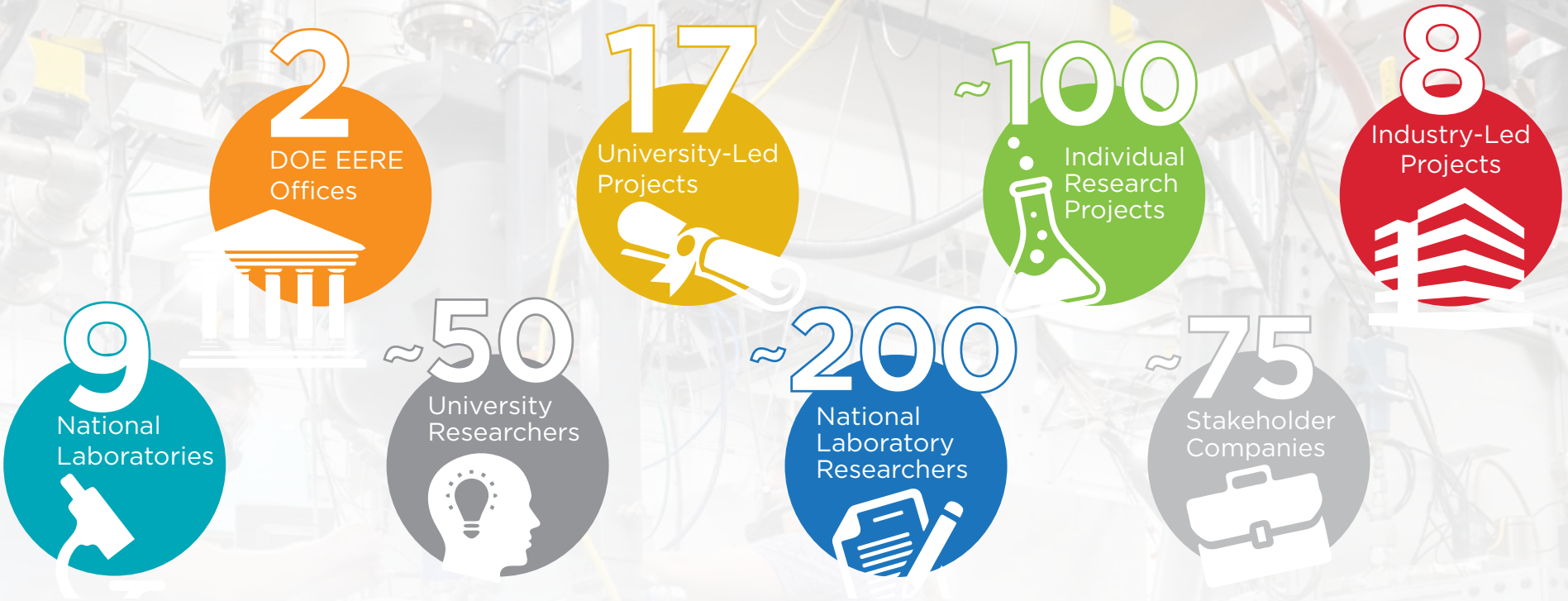
spark ignition (SI) ..... Combustion approach in which a fuel-air mixture is ignited by a spark plug

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

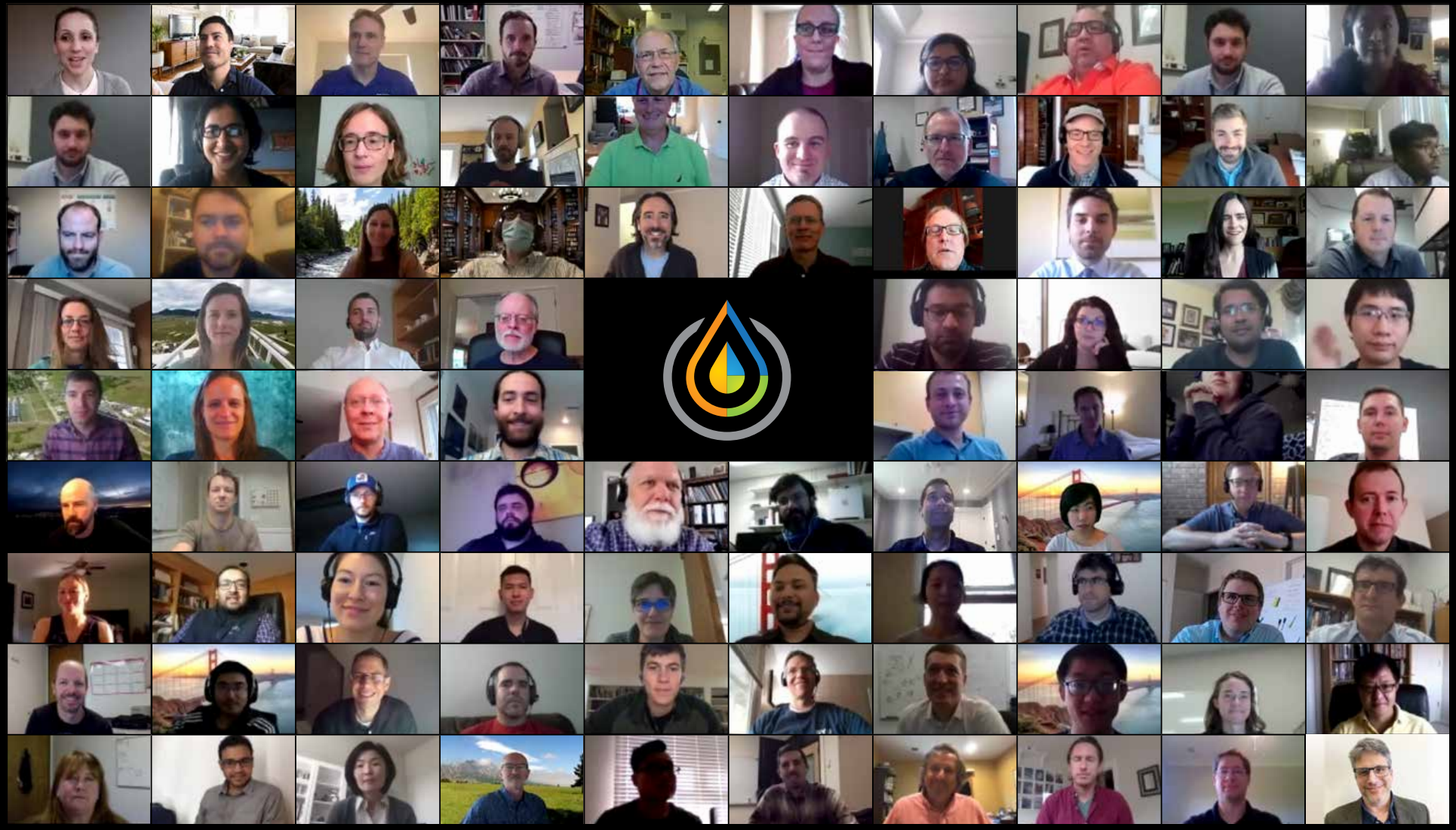
T50 ..... Temperature at which 50% of a fuel evaporates

T90 ..... Temperature at which 90% of a fuel evaporates

CO-OPTIMA BY THE NUMBERS



CO-OPTIMA TEAM MEMBERS



Hundreds of team members and stakeholders came together for more than one hundred virtual meetings throughout the year.

DOE/EE-2341
May 2021