U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

CO-OPTIMIZATION OF
FUELS & ENGINES

The Road Ahead

Toward a Net-Zero-Carbon Transportation Future

Findings and Impact | FY15–FY21

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Co-Optima breakthroughs reveal potential for improvements in transportation sources, energy efficiency, and environmental sustainability, while also benefiting the economy and the scientific process. These can ultimately help combat climate change, reduce dependence on petroleum from foreign sources, strengthen the energy market, and foster future innovation. More details can be found on the following pages and on the Co-Optima website: energy.gov/fuel-engine-co-optimization.

CO-OPTIMA IMPACT AT A GLANCE

Environmental Sustainability

Sustainable Domestic Fuel Sources

~25 viable bioblendstocks

GHG Reduction

>50% reduction for LD blendstocks with turbocharged SI combustion

>60% reduction for LD blendstocks with multimode combustion

>60% reduction for MD/HD blendstocks

Blendstock Criteria Pollutant Reduction for MD/HD vehicles

≥99% soot reduction with MCCI

≥80% NO_x reduction with MCCI

NO_x, soot & hydrocarbon reduction with ACI

Energy Efficiency

Light Duty

Up to 10% increase in engine efficiency with turbocharged SI combustion

Additional 9%–14% improvement in fuel economy with multimode combustion

Medium & Heavy Duty

Up to 4% increase in engine efficiency with ACI

Economic Viability

Fuels with cost-competitive prices of **$2.50-$4/GGE**

Up to 500,000 new biorefinery jobs

Maximum potential use of **1 billion tons of domestic biomass**

Lower emissions compliance costs for MD/HD diesel trucks

Scientific Process

>30 new tools for property prediction and simulation

New methods to more quickly & accurately assess **1,000s of blendstocks**

ACI = advanced compression ignition, GGE = gasoline gallon equivalent, GHG = greenhouse gas, HD = heavy duty, LD = light duty, MCCI = mixing-controlled compression ignition, MD = medium duty, NO_X = nitrogen oxide, SI = spark ignition

EXECUTIVE SUMMARY
Toward a Net-Zero-Carbon Transportation Future

Driving Deep Cuts in Transportation Energy Use and Emissions

The urgent need to decarbonize our transportation system—switching from petroleum-based fuels to cleaner, more sustainable energy sources—has become ever more apparent. While the nation is moving to rapidly boost production of electric vehicles, the transportation of goods and people will still rely heavily on gasoline and diesel fuel for decades to come.

In just a few short years, breakthroughs from the recently completed U.S. Department of Energy (DOE) Co-Optimization of Fuels & Engines (Co-Optima) initiative could improve cars' fuel economy by 10% for today's turbocharged engines and as much as 14% more for advanced engines using multiple combustion modes, compared to a 2015 baseline. At the same time, new bio-based fuel components could produce at least 60% fewer greenhouse gas (GHG) emissions than those generated by petroleum-based fuels for all on-road vehicles.

As of 2019, the number of cars and trucks powered by internal combustion engines (ICEs) continues to grow, accounting for more than 66% of all U.S. petroleum consumption and more than 25% of GHG emissions. Nearly 3 million new vehicles hit the nation's roads each year, adding to an existing fleet of more than 270 million. Annually, U.S. vehicles use more than 4 billion barrels of petroleum-based fuels and emit 1.6 billion tons of GHGs into the atmosphere.

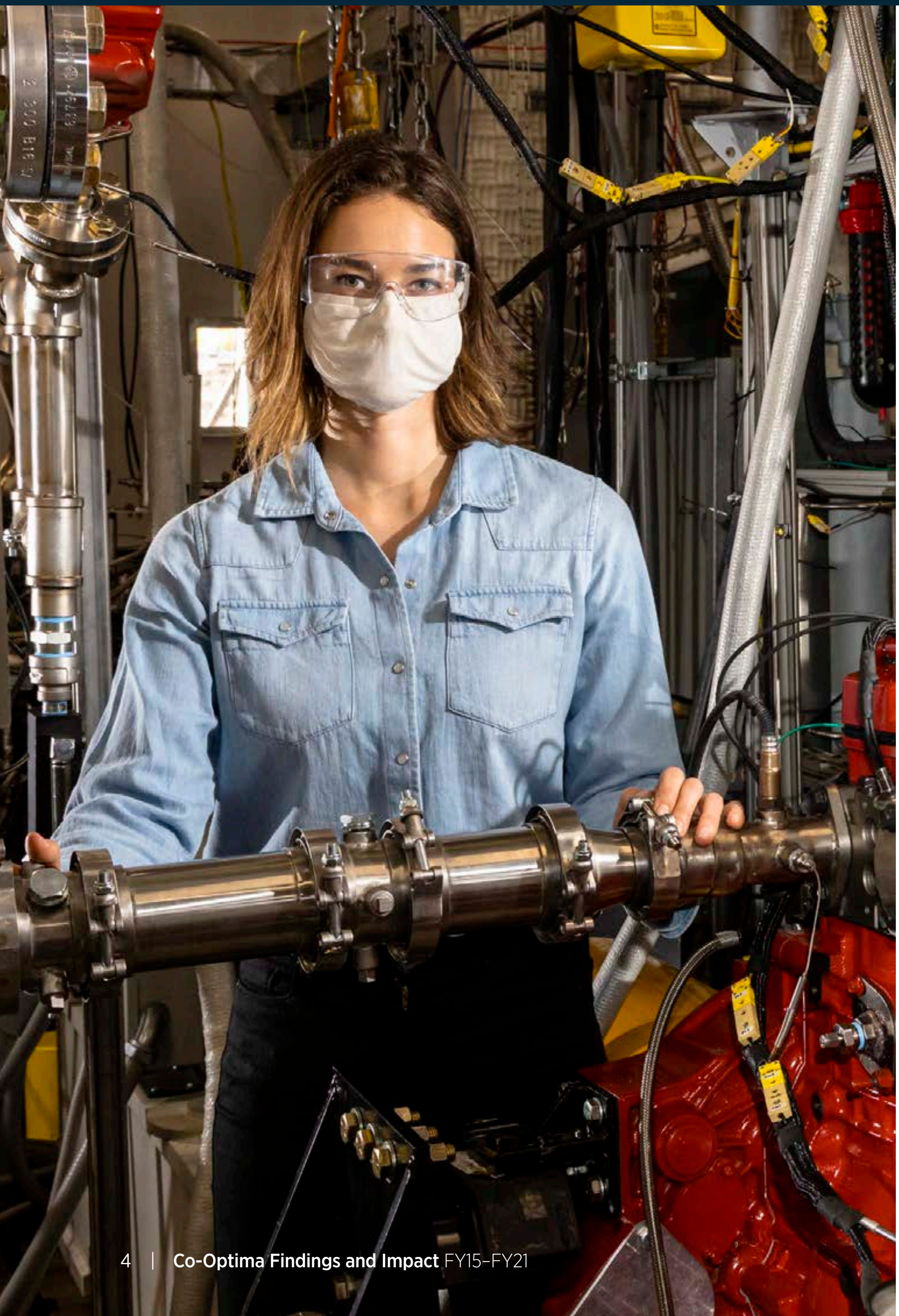
Recognizing that it would be a decade or more before greater numbers of zero-emission electric vehicles could make it off the assembly line, 6 years ago DOE launched the Co-Optima initiative. Top researchers from national labs across the country set out to develop clean, efficient, and affordable fuels and engines that could be brought to market sooner.

The immediate goal was to give American industry and policymakers the scientific knowledge, data, and tools needed to decide which alternatives could prove most viable and beneficial for drivers, businesses, and the environment. Ultimately, commercial adoption of Co-Optima innovations can make it possible to slash emissions, cut petroleum use, and contribute to ambitious national goals to reverse global warming.

Since the initiative's outset, Co-Optima researchers have made numerous breakthroughs with the potential to dramatically improve the performance of ICE vehicles. The team identified new low-emission, high-efficiency fuel-engine combinations for light-duty (LD), medium-duty (MD), and heavy-duty (HD) vehicles, using innovative methods and tools to expand understanding of combustion and fuel properties.

This report summarizes approaches, findings, and potential impacts of that landmark Co-Optima research. Detailed results are documented in more than 250 peer-reviewed journal articles, conference papers, and technical reports.

Photo: iStock



Photos: ORNL

A Collaborative, Cross-Disciplinary Approach

Success of the Co-Optima initiative relied on the strength of working together—in terms of both technologies and teams. Research examined how fuel and engine innovations could be engineered in tandem to maximize advances in vehicles' fuel economy and emissions, while spurring greater use of domestic renewable resources. At the same time, scientists, engineers, and analysts joined with other top minds from across the country, applying expertise from a wide range of disciplines to address research challenges.

While previous research focused on either the fuel or the engine, the Co-Optima team simultaneously examined potential fuels in combination with technologies for LD, MD, and HD engines. The initiative targeted near-term solutions with potential to improve gasoline and diesel fuels and engines in the marketplace today, as well as revolutionary longer-term innovations that could lead to the vehicles of tomorrow.

Through detailed modeling and analysis, goals were established for fuel economy savings, emissions reductions, production and operating costs, and other environmental and economic impacts. Co-Optima research explored options to meet these goals using blendstocks that can be produced from a wide variety of bio-based resources, added to conventional liquid fuels, and paired with a broad spectrum of conventional and advanced combustion regimes.

Co-Optima research extended the foundation of science and knowledge by determining those fuel properties critical to improving performance and reducing polluting emissions for a range of combustion approaches. Subsequent identification of specific blendstocks that can supply these fuel properties presents multiple options to improve the performance of engines for the full range of on-road vehicles and load conditions, factoring in road grade, resistance, and vehicle weight. Researchers also assessed factors such as materials compatibility, potential for production at commercial scale, and industry and consumer costs to identify blendstocks with the fewest barriers to adoption.

A collaborative effort made all of these discoveries possible. Led jointly by the Bioenergy Technologies Office and Vehicle Technologies Office of DOE's Office of Energy Efficiency & Renewable Energy, Co-Optima brought together more than 100 experts from 9 national laboratories and more than 40 industry and university partners.

Potential for Fuel Economy Improvements and Emissions Reductions

Co-Optima findings reveal potential for dramatic improvements in vehicle fuel economy and increases in the use of domestically sourced bio-based fuel for transportation, along with steep emissions reductions. This, in turn, has the potential to create new jobs and keep energy dollars in the United States, while decreasing costs for consumers and commercial operators at the pump. But most importantly, it holds promise for making a meaningful difference in the fight against climate change.

Near-term Co-Optima solutions might combine new low-carbon bioblendstocks with turbocharged spark-ignition (SI) combustion to improve LD vehicle efficiency at high loads, and with mixing-controlled compression ignition (MCCI) in conventional combustion strategies for MD and HD diesel trucks. Longer-term innovations might pair bioblendstocks with multimode approaches combining SI combustion and advanced compression ignition (ACI) to improve LD efficiency across drive cycles, and with other ACI strategies to improve low-load emissions and efficiency in MD and HD vehicles.

All top-performing blendstock candidates were shown to reduce life cycle GHG emissions by at least 50% and have the potential to be produced at a commercial scale. Combined with advanced multimode combustion strategies, the blendstocks improved fuel economy by 9% to 14%, or by 10% for turbocharged SI engines.

The top-performing MCCI blendstocks also delivered reductions in harmful particulate criteria emissions, and enabled changes in engine operation that reduced nitrogen oxide production. The most promising blendstock candidates can be produced from a variety of domestic resources, including nonfood agricultural waste, forestry byproducts, used cooking oil, livestock manure, wastewater residuals, and more.

Bridging from Low-Carbon to No-Carbon Transportation

What comes next for fuel and engine research? The answer lies at the intersection of potential Co-Optima solutions with transitions in national and global market, policy, and research priorities.

The world has changed since the Co-Optima initiative started 6 years ago. Reducing GHG emissions is even more urgent. Electric vehicles are anticipated to gain a significant share of the LD market in the next 15 years, and renewable electricity generation is growing rapidly. Greater recognition of environmental justice considerations, including the disproportionate impact of transportation pollutant emissions on underserved communities, is beginning to play a larger role in research, development, and deployment decisions.

Photos: ORNL

Even as more electric cars are introduced and charging infrastructure is expanded, it will still take decades to turn over the entire LD vehicle fleet. Due to weight and operational patterns, trucks pose additional challenges to electrification, and are projected to run on liquid fuels for even longer. More sustainable, low-emission, high-efficiency vehicles using ICEs and liquid fuels such as those identified by Co-Optima will play an important role in reducing GHG emissions during that transition. Beyond ground transportation, approaches pioneered by Co-Optima point the way to sustainable fuels, improved efficiency, and reduced GHG emissions for air, marine, and rail transportation as well.

Finally, it is not an option to delay smaller-scale, near-term reductions while the search continues for a perfect solution—it is critical to begin reducing carbon emissions today. The incremental yet meaningful improvements identified by Co-Optima research can be implemented in the coming years, while making progress toward a longer-term net-zero-carbon-emissions transportation system based on more universal adoption of electric vehicles. A supportive economic and policy framework can ensure that these changes maintain momentum toward full decarbonization, reduce reliance on non-domestic energy sources, and reduce exposure to pollution for all Americans.

The successes of Co-Optima represent a beginning, not an end. The eventual transition to a net-zero-carbon-emissions transportation system will require concerted efforts led by industry, with continued involvement of university and national laboratory researchers over the coming decades. Co-Optima solutions provide a bridge from today's petroleum-dependent transportation system to cleaner bio-based fuels and an emissions-free tomorrow.

See the following pages for more detail on the most significant Co-Optima accomplishments. Additional information can be found on the Co-Optima website: energy.gov/fuel-engine-co-optimization.

WHAT'S NEXT?
Future research can build on Co-Optima findings and advance national goals to reverse climate change with contributions to:

- Fully decarbonizing the transportation system.
- Co-optimizing engines with 100% sustainable fuel replacement solutions.
- Addressing hard-to-electrify transportation sectors, including air, marine, off-road, and rail.


Photo: NREL

TECHNICAL RESEARCH FINDINGS & IMPACTS

Combined Approaches to Maximize Results

Jump-Starting Viable Solutions with Foundational Research

Co-Optima set out to make dramatic improvements to fuels and engines by examining the two research areas in tandem. By focusing on the fuel properties of bioblendstocks—components designed to be blended into gasoline or diesel fuel—in relation to a range of combustion strategies, the initiative discovered ways to deliver greater efficiency and lower emissions with both conventional and advanced engines.

The fuel-engine combinations identified by Co-Optima research can act as an effective bridge between conventional petroleum-fueled vehicles and a future fleet dominated by electric vehicles, supporting the national transition to a net-zero-carbon-emissions transportation system. Combined with other technology advancements already underway, these Co-Optima breakthroughs can help improve fuel economy by 10%–20% for light-duty (LD) vehicles, slash engine-out criteria pollutant emissions by as much as 99% for medium-duty (MD) and heavy-duty (HD) engines, and reduce greenhouse gas (GHG) emissions related to new blendstocks by 50% or more for all on-road vehicles.

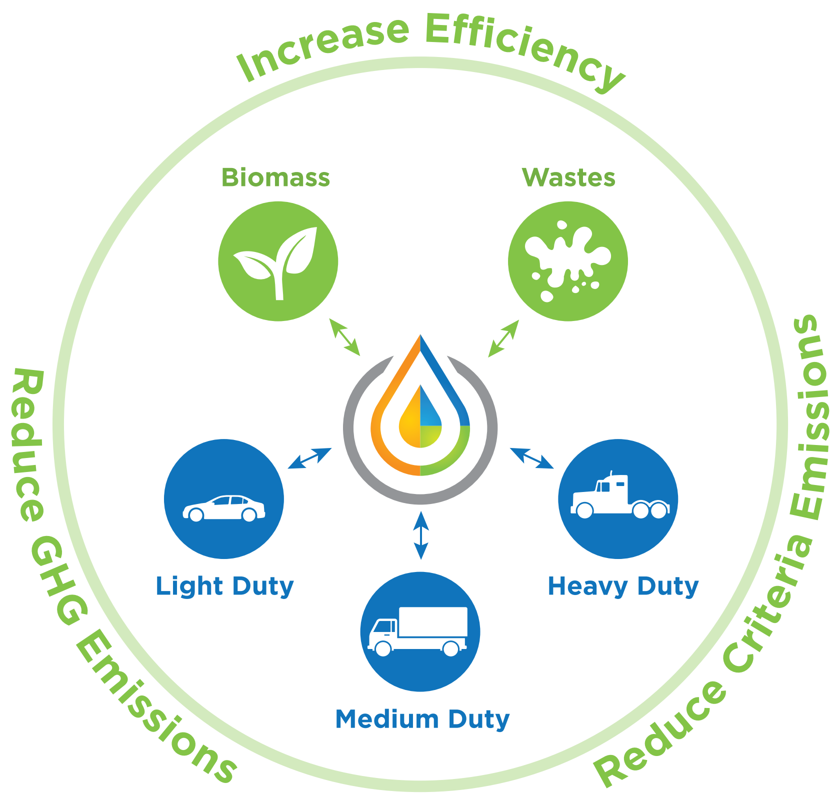
The goal of this foundational research was to help catalyze commercialization of these solutions, making it possible for industry to bring viable products to market sooner.

Exploring the Full Range of On-Road Vehicles and Combustion Technologies

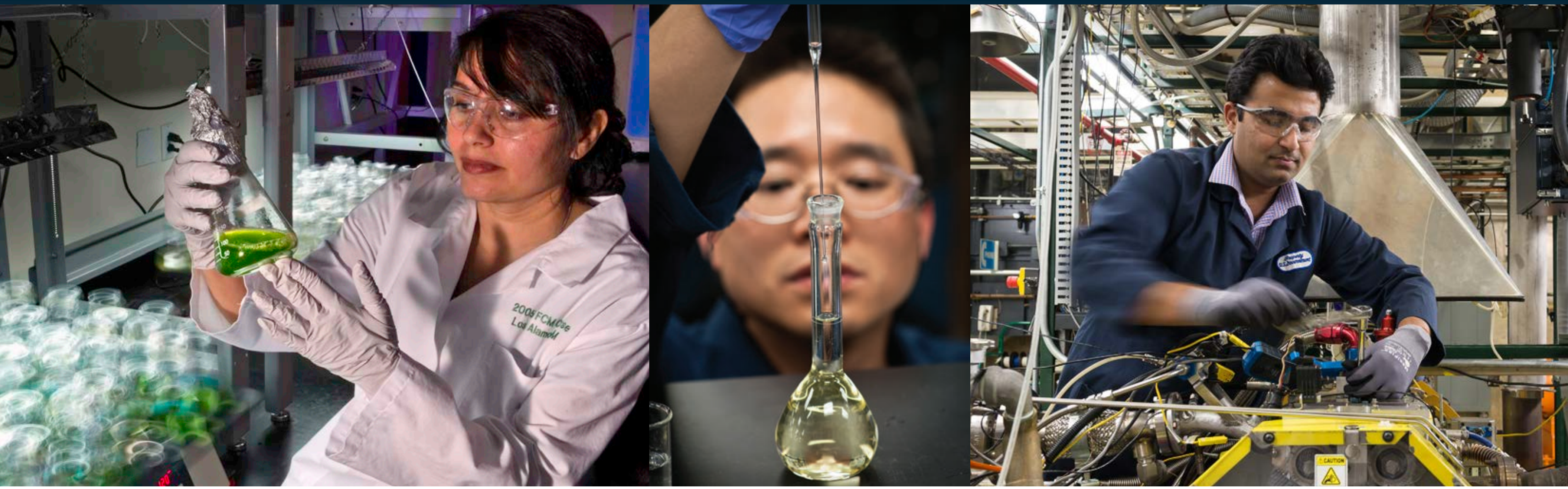
Laboratory fuel and engine research was combined with analysis to identify and address economic, environmental, and performance barriers and drivers for adoption, evaluating the sustainability of feedstocks, properties of candidate blendstocks, and options for conventional and new combustion approaches. Co-Optima research included experiments with single-cylinder, multicylinder, and optical engines; fuel-spray vessel experiments; laboratory bench-scale ignition and fuel reactivity experiments; computational chemical-kinetics combustion simulations; computational fluid dynamics engine combustion modeling; and vehicle-level drive-cycle simulations.

Researchers explored solutions for the full range of on-road vehicles, from LD cars to HD freight trucks. For LD transportation, the initiative examined turbocharged spark-ignition (SI) engines and multimode engines (which combine SI and compression ignition). The initiative evaluated conventional diesel combustion and a ducted fuel injection modification, along with other advanced combustion approaches for MD and HD vehicles. Co-Optima's approaches can also be applied to develop more efficient, lower-GHG-emissions solutions for other transportation modes such as air, marine, and rail.

Fuel-Engine Co-Optimization Delivers Benefits for Multiple Transportation Modes



Combined fuel and engine research can provide advanced high-efficiency, low-emissions options for a range of on-road transportation modes.



Photos: LANL, NREL, ANL (left to right)

Revealing Fuel Properties Needed to Optimize Benefits

Concurrent with this engine research, the Co-Optima team worked to identify viable bioblendstocks, production pathways, and finished-fuel blending properties. Researchers screened and evaluated more than a thousand options to determine their potential to improve the performance of today's engines, meet the demands of future engines, cut emissions, and determine potential to produce at the scale and cost required for commercial market success.

The team considered blendstocks that can be produced from the potential billion-ton annual supply of domestic biomass resources. Promising sources for bioblendstocks span a range of sources including sustainable energy crops such as switchgrass; forestry and agricultural crop waste; livestock manure; municipal solid and wet waste; waste fats, oils, and greases; and algae. The team used a series of sophisticated modeling tools and algorithms to identify blendstock candidates with properties most likely to deliver needed performance, environmental, and economic attributes.

More details on the most significant Co-Optima foundational discoveries and findings can be found in the following sections. Additional information on Co-Optima research, along with many of the tools and data sets mentioned in this report and a searchable publications database, can be found on the initiative website: energy.gov/fuel-engine-co-optimization.

FOUNDATIONAL DISCOVERIES

Revealing the Scientific Underpinnings of Fuel-Engine Co-Optimization

Setting the Stage to Improve Efficiency and Reduce Emissions

Crosscutting by design, the Co-Optima initiative set out to develop fuel and engine combinations that work together to maximize efficiency, environmental, and economic benefits. Co-Optima researchers applied fundamental principles to fuel and engine research for light-duty (LD), medium-duty (MD), and heavy-duty (HD) vehicles, focusing on blendstocks to be combined with petroleum gasoline and diesel fuels. These core scientific approaches guided the entire Co-Optima research effort, spanning multiple disciplines to ultimately identify the most promising fuel and combustion options and provide a foundation for future research.

Two hypotheses set the stage for the Co-Optima initiative. The central engine hypothesis states that engine architectures and combustion strategies can provide higher thermodynamic efficiencies than those available from today's internal combustion engines, when combined with new fuels designed to maximize efficiency and operability across a wide range of speeds and loads. The central fuel hypothesis theorizes that fuels with certain properties critical to improving efficiency and emissions for a given engine architecture will provide comparable performance, regardless of chemical composition.

These governing hypotheses guided researchers in developing screening criteria and evaluating thousands of candidate mixtures and molecules. The hypotheses were also applied to investigate multiple combustion modes, including turbocharged spark-ignition (SI) approaches for LD engines, mixing-controlled compression ignition (MCCI) for MD and HD engines, and advanced compression-ignition (ACI) and multimode approaches for all three types of vehicles burning gasoline and diesel fuels. ACI combustion, a continuum of combustion modes controlled by the degree of fuel and air mixing in the cylinder at the start of combustion, offers the greatest potential improvements in efficiency and reductions in criteria pollutant emissions, well beyond those found with SI or MCCI combustion approaches.

Prioritizing R&D with a Tiered Approach to Blendstock Screening

A major portion of Co-Optima research focused on identifying blendstocks that can be produced from a variety of renewable domestic biomass and waste resources and added to conventional liquid fuels to improve fuel economy and reduce emissions. Using a process streamlined by the fuel and engine hypotheses, a systematic study identified a broad range of blendstocks as feasible options based on their fuel properties.

MAJOR FOUNDATIONAL DISCOVERIES AND IMPACTS

- Established central engine and fuel hypotheses to guide research activity.
- Developed engine efficiency merit function for turbocharged SI combustion and target values of fuel properties for other combustion modes.
- Evaluated thousands of molecules and mixtures through tiered screening to identify 10–15 most promising blendstocks each for diesel and gasoline fuels.
- Advanced understanding of chemical kinetics, particularly their effects on autoignition and soot formation.
- Uncovered new insights into fuel molecular structure-property relationships to predict fuel properties and identify new blendstock candidates.
- Assessed interplay of candidate blendstocks with multiple combustion approaches.

Researchers first conducted high-level experimental and computational screening based on a subset of critical properties (boiling point, freezing point, ignition quality, and more) to determine which among thousands of potential blendstocks met the technical criteria to be used in fuel. In the second step, the team evaluated which of the hundreds of blendstocks that made it through the first screening could enable increased engine performance, prove viable for commercial production from biomass, reduce life cycle carbon dioxide emissions, and overcome major barriers to widespread market introduction, such as materials compatibility. The final step of blendstock research focused on assessing the remaining candidates for co-optimized performance in an actual engine.

Top-performing blendstocks were evaluated according to the combustion modes under consideration. For LD turbocharged SI and SI/ACI multimode engines, Co-Optima researchers relied on an efficiency merit function, a mathematical formula, to identify blendstocks with the most promise to deliver the targeted greenhouse gas emissions and efficiency results. Based on the central engine hypothesis, the merit function was key to understanding the co-optimization potential of candidate blendstocks and was used to guide experiments.

The complex variables involved in reducing criteria pollutant emissions from MCCI engines and delivering wider operability with ACI engines ruled out the development of a comparable merit function to assess blendstock options for those engines. Instead, researchers identified a set of additional fuel properties related to operability and emissions that played a critical role in predicting the performance of blendstocks in MD and HD MCCI and ACI engines.

Further analyses assessed technology readiness, environmental impact, and economic feasibility for the many combinations of blendstock, combustion, and vehicle options.

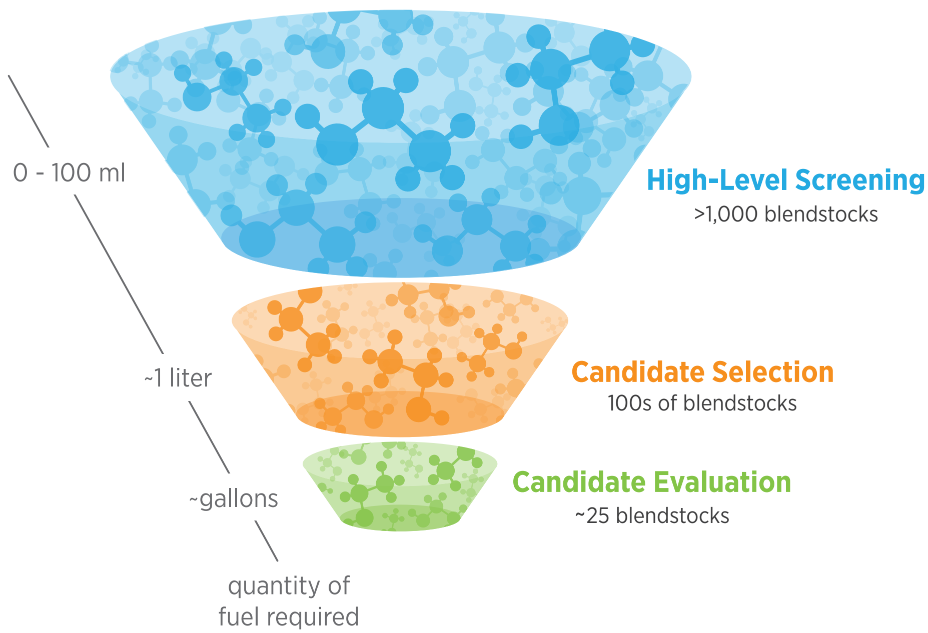
Tying Fuel Properties to Chemical Structure Through New Insights

Evaluating blendstocks requires measuring or predicting their critical fuel properties. Co-Optima research led to a new understanding of the relationships between chemical structures and fuel properties. Chemical structure-fuel property relationships tie molecular composition and bonding arrangements to the physical and combustion properties of fuels. These relationships can be used to predict the performance of new candidate molecules and simple mixtures and help understand the behavior of more complex blends. New Co-Optima insights helped dramatically improve the scope and fidelity of combustion kinetic simulations that are critical for predicting fuel behavior.

Co-Optima researchers developed an understanding of structure-property relationships for a comprehensive set of properties important for fuel performance and combustion, including autoignition, sooting propensity, thermophysical behavior, and others. This information helped accelerate the identification of the most promising candidates through the rapid screening of large numbers of blendstocks.

The team determined structure-property relationships through empirical correlations, chemical reaction mechanisms and rates, simulations, and machine learning. Machine learning was used to calculate initial conditions such as bond dissociation energy, and quantum mechanics theory was used to evaluate the feasibility of proposed mechanisms and calculate reaction rates. These enabled simulations of autoignition, combustion, and soot formation, delivering many new insights that will inform future fuel design.

New Methods Result in a More Efficient and Effective Blendstock Screening Process



Approximately 25 blendstocks with demonstrated performance advantages were identified from a pool of thousands of candidates. Research approaches using new computational methods and small volumes of fuel made it possible to evaluate candidates quickly and accurately.

LIGHT-DUTY FINDINGS

Potential for 10% or Greater Fuel Economy Gains and 60% Greenhouse Gas Emissions Cuts

Tackling Transportation's Greatest Source of Energy Use and Emissions

Each year in the United States, light-duty (LD) vehicles including light trucks and passenger vehicles move people and goods about 3 trillion miles, consuming 57% of all energy used for transportation and producing 58% of transportation-related greenhouse gas (GHG) emissions.

Co-Optima research revealed that these LD vehicles can be designed to operate more efficiently. In fact, improvements of 10% or more are possible by combining current and advanced engine designs with higher-performing sustainable fuels produced from renewable, domestic, non-petroleum resources. This is beyond an already expected 25% improvement in fuel economy for engine-only advances anticipated in the next few years. At the same time, co-optimized fuels and engines have the potential to reduce emissions of carbon dioxide and other pollutants by 60% or greater relative to those of petroleum-based fuel.

Automakers already offer sophisticated high-efficiency turbocharged engines for LD vehicles, but fuel properties constrain the maximum efficiency of these engines, which are still powered primarily by petroleum-based fuels. Co-Optima researchers explored how to maximize performance and minimize emissions through a systematic understanding of the relationships between fuel properties and combustion approaches.

In the past 6 years, Co-Optima researchers identified opportunities to increase the efficiency of turbocharged spark-ignition (SI) engines by up to 10%. The initiative also investigated how even greater efficiencies—as much as an additional 14%—can be delivered with new advanced multimode engines that use different methods of ignition and combustion depending on engine needs. Due to the complexities of multimode vehicle operation and drive cycles, further experiments and analysis are needed to determine precisely how much more fuel economy multimode operation might offer on top of that delivered by turbocharged SI.

For both types of engines, combustion research focused on determining fuel properties critical to greater engine efficiency, cleaner combustion, and lower pollutant emissions. Concurrent with engine research focused on combustion approaches, the Co-Optima team also sought to identify viable bioblendstocks, production pathways, and finished-fuel blending properties.

Researchers screened and evaluated hundreds of gasoline-boiling-range blendstocks that could be generated from biomass and waste. These efforts determined which blendstocks could provide the fuel properties needed to improve the performance of today's LD engines, meet the demands of future engines, cut emissions, and be feasible to produce at the scale and cost required for commercial success.

MAJOR LIGHT-DUTY FINDINGS AND IMPACTS

Up to 10% Turbocharged SI Fuel Economy Gain

Identified critical fuel properties and potential fuel economy gains for turbocharged SI engines:

- Provided target values of critical fuel bioblendstock properties.
- Identified RON and S as most important fuel properties.
- Identified importance of blending synergistically for RON.
- Developed a merit function to evaluate properties needed in candidate blendstocks for optimal engine performance.

Additional 9%–14% Gain with Multimode Approaches

Identified critical fuel properties and potential fuel economy gains for multimode engines:

- Found multimode fuel property requirements to be compatible with those for turbocharged SI.
- Confirmed additional fuel economy gains are possible for multimode engines.
- Identified pathway to fuel economy gains with lower RON and S than required for high-efficiency turbocharged SI engines.

Blendstock Options to Deliver Performance Advantages

Identified bioblendstocks with greatest potential to improve fuel economy while reducing emissions:

- Determined alcohols and olefins to be most promising bioblendstock candidates for both turbocharged SI and multimode engines.
- Identified 9 molecules and mixtures with the potential to reduce GHG emissions by 60% or more when used in turbocharged SI or multimode engines.
- Discovered that most candidate blendstocks offer favorable economic metrics, with 7 that meet target prices ≤$4/GGE.

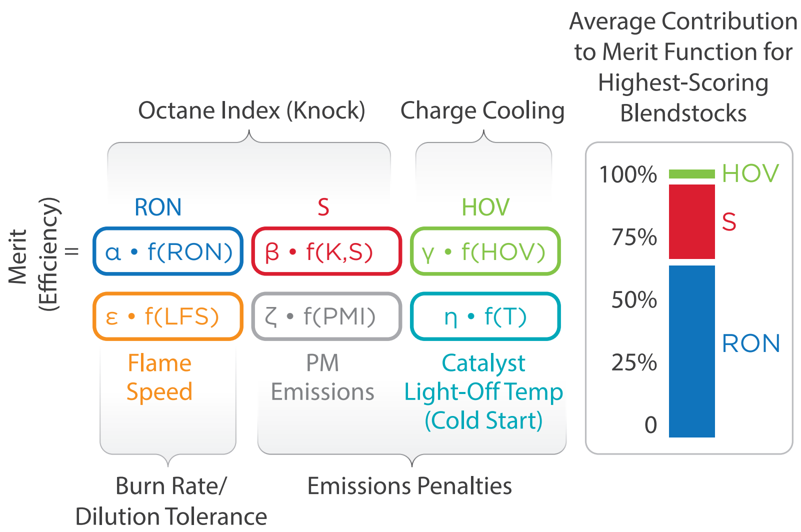
Photo: iStock

Boosting the Efficiency of Turbocharged Engines

Engine-combustion research quantified the impact of 6 different fuel properties on engine efficiency for turbocharged SI engines: research octane number (RON), octane sensitivity (S), heat of vaporization (HOV), flame speed, particulate matter (PM) index, and catalyst light-off temperature. RON and S were found to be the most important properties, allowing the use of efficiency-enhancing approaches including higher compression ratio, more aggressive engine downsizing, and intake-pressure boosting.

Computations using a mathematical formula termed a merit function were the key to screening candidate bioblendstocks and identifying properties with the greatest potential performance paybacks. The Co-Optima merit function quantifies the impact of fuel properties, providing the most detailed correlation developed to date relating fuel properties and engine efficiency. This approach makes it possible to explore how changes in key fuel properties can trigger trade-offs related to engine efficiency.

Merit Function Quantifies Fuel Properties' Impacts on Engine Efficiency



The merit function (left) quantified the impact of RON, S, HOV, flame speed, PM emissions, and catalyst light-off temperature. The bar graph (right) shows the average contribution of RON, S, and HOV to the overall efficiency delivered by the highest-scoring boosted SI blendstocks studied.

Delivering Higher Efficiency with Multimode Engines and Less Extreme Changes in Fuel Properties

Multimode SI engines can use more efficient combustion methods at low loads and speeds, where engine efficiency drops off for turbocharged SI engines. Engine loads increase when the vehicle is accelerating, climbing a hill, or carrying more weight. Co-Optima researchers analyzed spark-assisted compression ignition, stratified-charge SI, pre-chamber lean SI, and advanced compression-ignition (ACI) combustion approaches to determine desirable fuel property targets for these modes.

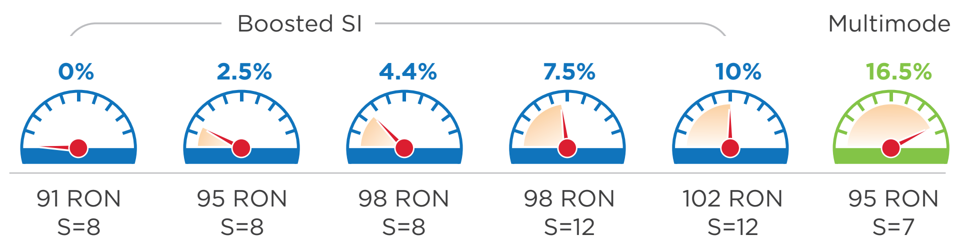
Ultimately, researchers identified cases where the understanding of critical fuel properties was incomplete, indicating a need for more foundational research. Extensive additional research determined that high RON and S are vital to high efficiency for all these LD combustion modes, but multimode approaches can deliver significantly greater efficiency with fuels exhibiting lower RON and S values than required for the most efficient turbocharged SI engines.

Co-Optima multimode engine modeling showed potential efficiency gains 9%–14% greater than those found with turbocharged SI engines. This amounts to a modeled 16.5% fuel economy improvement using SI/ACI multimode combustion approaches and fuel properties consistent with premium gasoline.

Co-Optima research also identified several blendstocks that demonstrated synergistic blending and what is known as the hyperboosting of RON. When properties blend in an approximately linear fashion, the properties of the resulting fuel can be readily calculated based on a simple linear combination of the properties of its components. Nonlinear behavior results in fuel properties that are either higher (synergistic)—which is the case for hyperboosting of RON—or lower (antagonistic) than a linear calculation would predict. Blendstocks including alcohols, furans, olefins, and cyclic ketones that demonstrate synergistic blending behavior have significant potential to improve engine efficiency for conventional and advanced combustion modes.

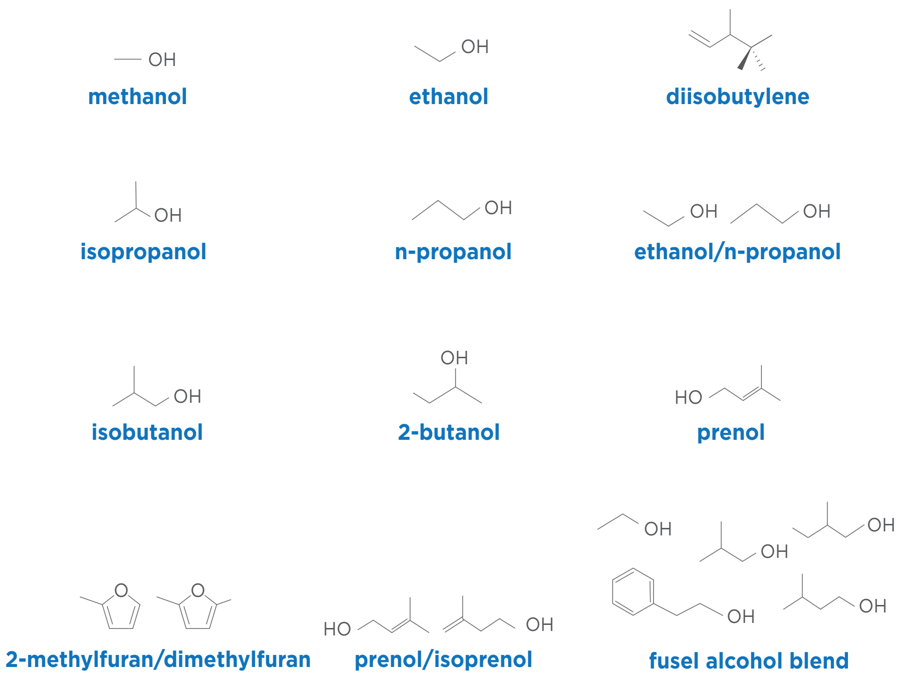
Photos: LBNL

Changing Fuel Properties Can Increase LD Engine Efficiency



Merit function estimates of turbocharged SI efficiency increases and drive-cycle modeling estimate of multimode efficiency reflect the increase enabled by changes in RON and S.

Top LD Blendstock Candidates Reduce GHG Emissions and Improve Fuel Economy



Screening identified 12 blendstocks that impart the desired properties to a petroleum base fuel for boosted SI and multimode engines.

Discovering Bioblendstocks with Improved Properties

Co-Optima researchers identified a set of 12 bioblendstocks compatible with turbocharged SI and multimode combustion strategies that also showed potential for reducing life cycle carbon emissions and achieving high market penetration. Co-Optima evaluated blendstocks that would be combined with a base gasoline fuel in volumes up to 30%. Alcohols and olefins appeared to be the most promising candidates for both LD combustion approaches. Methanol, 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), diisobutylene, and a methylfuran/dimethylfuran mixture (40/60 by weight) all met the performance, efficiency, and environmental criteria. Two other blendstocks, prenol and a fusel alcohol blend, reduced GHGs by more than 50% in comparison to fossil fuels.

Producing these blendstocks from low-net-carbon feedstocks dramatically reduces life cycle GHG emissions. Of the candidate blendstocks, lignocellulosic ethanol is already a market fuel, and isopropanol, n-propanol, isobutanol, diisobutylene, and the ethanol/n-propanol mixture have the fewest barriers to adoption. The candidate blendstocks offer favorable economic metrics, with potential production costs for 7 blendstocks of $4 or less per gasoline gallon equivalent (GGE).

Photo: ANL

Potential for Up to 4% Fuel Economy Gains and Greater Than 60% Greenhouse Gas Emission Cuts

Reducing Diesel Engine Energy Consumption and Pollution

Medium-duty (MD) and heavy-duty (HD) trucks haul 10 billion tons of cargo across the United States every year. These vehicles account for 24% of all transportation-related energy use and greenhouse gas (GHG) emissions.

The diesel-fueled engines typically found in commercial freight trucks deliver impressive power and operate with high thermal efficiency, but require costly and complex control systems to meet emissions regulations. The Co-Optima team identified ways to improve MD and HD engine efficiency by up to 4% and maintain fuel energy density, cut GHG emissions by 60%, and virtually eliminate soot production, while making emissions compliance more affordable.

This research spanned mixing-controlled compression-ignition (MCCI) and advanced compression-ignition (ACI) combustion approaches. MCCI technology is used in today's commercial diesel engines. Potentially transformative ACI approaches can achieve even higher thermodynamic efficiency while yielding lower emissions.

The already high thermal efficiency of MCCI combustion means that further advances in MCCI engines offer only modest additional efficiency gains. This led Co-Optima researchers to focus on improving MD and HD truck performance by identifying sustainable new blendstocks, engine technologies, and combustion approaches capable of reducing environmental impacts.

MAJOR MEDIUM-DUTY AND HEAVY-DUTY FINDINGS AND IMPACTS

Up to 4% Fuel Economy Gain with ACI Approaches
Co-optimized specially designed fuel to deliver simultaneous efficiency and emissions improvements:

- Designed fuel containing 40% bioblendstocks tailored to ACI engine co-optimization.
- Combined fuel with low-temperature gasoline combustion to demonstrate ≤4% fuel economy gain.

Dramatic Reductions in GHG and Criteria Emissions
Identified combustion and blendstock combinations to reduce emissions:

- Demonstrated the ability of bioblendstocks to cut life cycle GHG emissions by >60%.
- Determined DFI combined with lower-sooting blendstocks can reduce engine-out soot production by ≥99%.
- Cut NO_X emissions by ≥90% through ACI/MCCI multimode combustion approaches.
- Reduced NO_X and soot production using lower-sooting blendstocks in a diesel engine.

Blendstock Options to Deliver Performance Advantages
Identified top 13 bioblendstocks with greatest potential to improve operability while reducing emissions:

- Identified blendstocks offering improved cold-temperature operability, increased cetane number, and reduced sooting potential, while minimizing decrease in energy density.
- Discovered that most candidate blendstocks offer favorable economic metrics, with 4 that meet target prices ≤$4/GGE.

Cutting Emissions with New Bioblendstocks

Co-Optima researchers identified 13 sustainable diesel-boiling-range blendstock options. All of these top blendstock candidates have the potential to decrease life cycle GHG emissions by more than 60% and reduce criteria pollutants.

Although the complexity of variables meant that no merit function could be constructed to link fuel properties to performance in an MCCI engine, fuel properties key to improving operability and decreasing criteria pollutant emissions were identified. They included cetane number, cloud point and pour point, soot propensity, flash point, and energy density.

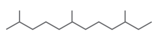
Of the many blendstocks providing target values of these fuel properties, hydrocarbons present the fewest barriers to market entry. Although some esters may have diesel-engine compatibility issues (especially at high blending levels), they are already widely used in biodiesel at lower blending levels (usually less than 5%). Ethers have the highest barriers to market entry, with challenges related to compatibility, oxidative stability, and other properties. Most candidate blendstocks offer favorable economic metrics, with 4 meeting target prices of $4 or less per gasoline gallon equivalent (GGE).

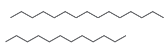
Advanced approaches using a different set of gasoline-range blendstocks, such as those developed for light-duty vehicles, could improve engine efficiency by up to 4% compared to the baseline MCCI diesel engine, while producing very low soot and nitrogen oxide (NO_X) emissions. Co-Optima researchers designed a furan-based fuel bioblendstock with the high research octane number, octane sensitivity, phi sensitivity, and other properties needed to deliver these improvements.

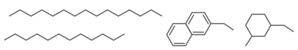
Photo: iStock

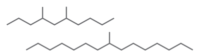
Top MD and HD Blendstock Candidates Offer GHG Reductions and Fuel Property Improvements

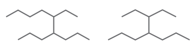
Hydrocarbons

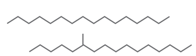

farnesane


Fischer-Tropsch diesel

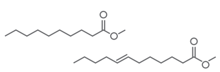

hydrothermal liquefaction oil from wet waste, algae, and algae-wood blends

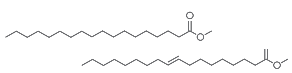

isoalkanes made from ethanol

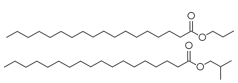

isoalkanes via volatile fatty acids from food waste


hydroprocessed esters and fatty acids (renewable diesel)

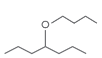
Esters

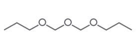

short-chain esters from oilseed crops

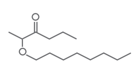

fatty acid methyl esters/biodiesel

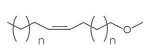

fatty acid fusel esters

Ethers


4-butoxyheptane


polyoxymethylene ethers (POMEs)


alkoxyalkanoates


fatty alkyl ethers

Screening identified 13 blendstocks that impart improved cetane number and low-temperature operability. These blendstocks produce little soot, provide energy content comparable to that of petroleum-based fuel, and have the fewest barriers to commercial introduction.

Photo: iStock

Exploring the Potential of Advanced Engine Technologies

One of the primary challenges facing MD and HD MCCI engines is compliance with NO_X emission standards at low engine loads. Low exhaust temperatures make it difficult for the emissions control catalysts to work effectively.

Co-Optima researchers investigated a multimode strategy that relied on a different ACI combustion approach, using diesel-boiling-range fuels to reduce engine-out NO_X emissions under light loads and efficient MCCI operation under high loads. This strategy was shown to reduce NO_X emissions tenfold. Several of the top 13 bioblendstocks were tested and proved compatible with this ACI strategy, producing comparable NO_X reductions and further reductions in hydrocarbon emissions.

Co-Optima researchers also developed a new ducted fuel injection (DFI) HD engine technology that enhances the mixing of fuel and air prior to combustion, minimizing the fuel-rich zones prone to soot formation. DFI alone can decrease engine-out soot emissions by a factor of 10 compared with those of today's MCCI engines. Combining DFI technology with a low-sooting Co-Optima blendstock candidate can cut those emissions even more, by a total factor of 100.

Fuel and engine combinations that produce fewer NO_X and soot emissions may also help diminish MCCI engine operating costs by reducing how frequently particulate filters require cleaning. Some of the top blendstock candidates can decrease MCCI engine-out soot emissions, as well as NO_X emissions, by enabling higher levels of exhaust gas recirculation. This in turn makes it possible to use less diesel emission fluid, resulting in a lower total cost of ownership that could contribute to greater adoption.

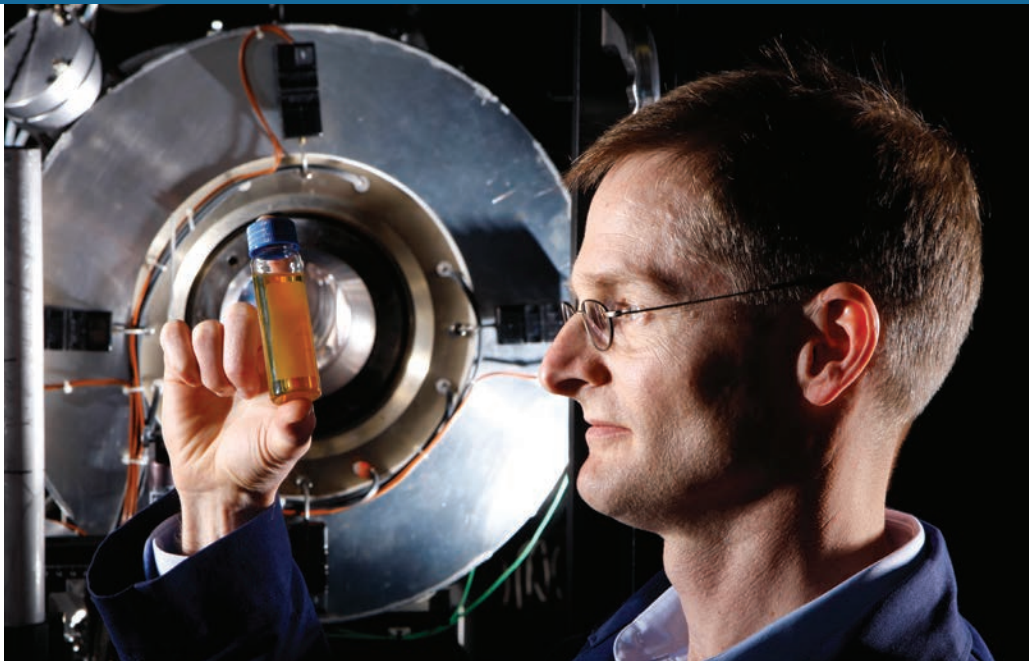
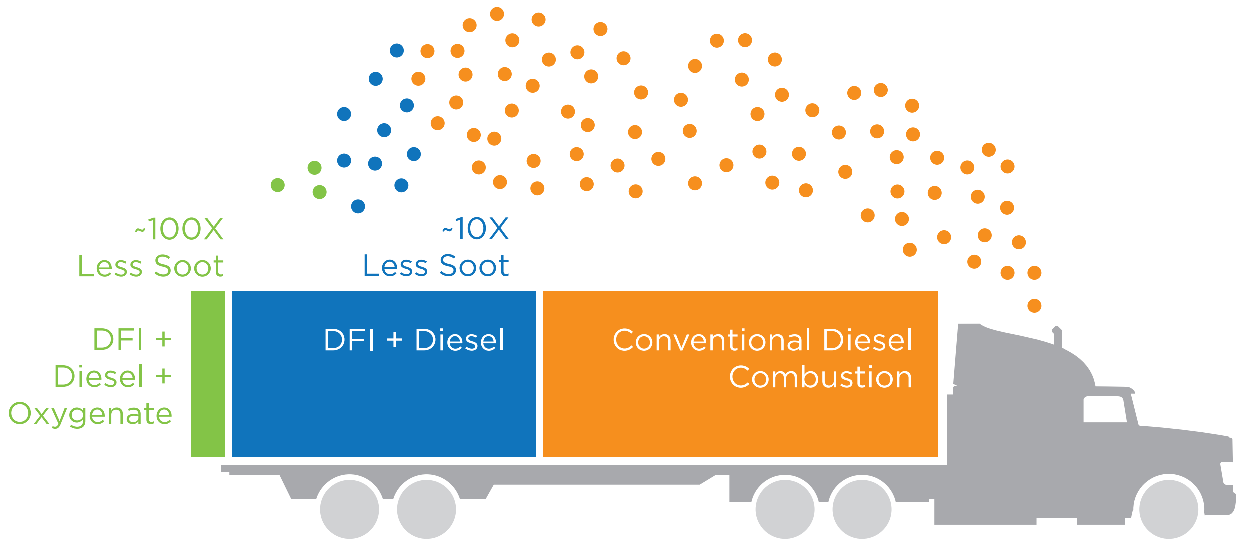


Photo: SNL

DFI and Sustainable Fuels Can Reduce Soot Production



DFI reduces in-cylinder soot production by ~90% compared to conventional diesel combustion. Combining DFI with a blend of 25% sustainable oxygenate blendstock and diesel fuel reduces soot by ~99%.

ANALYSIS FINDINGS

Quantifiable Opportunities for Scalable, Affordable, Clean, and Efficient Solutions

Moving Innovations Beyond the Laboratory

Overcoming hurdles in engine design and fuel formulation are just the initial steps in moving co-optimized transportation solutions from laboratories onto the nation's roads. Making sure new fuels and engines can be scaled up for commercial production, will be compatible with fueling infrastructure and automotive components, and can be produced at costs that are competitive for both industry and consumers are all vital factors in bringing cleaner, more efficient transportation solutions to market.

Co-Optima techno-economic and life cycle analyses determined key economic drivers for new fuel and engine technologies, identifying which bioblendstocks could reduce greenhouse gas (GHG) emissions the most at a given target production cost. Research also indicated that certain bioblendstocks with improved research octane number (RON), octane sensitivity (S), sulfur content, and cetane number (CN) properties could provide refineries with additional economic benefits.

Researchers applied benefits analyses to determine the possible value commercial adoption could deliver to both consumers and industry. These findings point the way for automakers, fuel producers, and other transportation sector decision makers to bring these new bioblendstocks and vehicle technologies to market.

Not only did Co-Optima experimental research reveal potential for significant gains in fuel economy and reductions in emissions, but the team's analyses also provided quantifiable estimates of those gains. Analyses also indicated that the bioblendstocks identified through Co-Optima could benefit automotive manufacturers' and fuel producers' business operations and profitability, along with providing new means to meet increasingly demanding fuel and emissions specifications.

Steering Early-Stage Evaluation with Upfront Analysis

Promising biofuel pathways were identified based on environmental, economic, and scalability considerations. Analysts worked closely with researchers to identify which potential bioblendstocks could meet volume, cost, and GHG emissions targets. This iterative process analyzed more than 50 candidates based on fuel properties and performance characteristics to identify approximately 25 low-carbon bioblendstocks that could be produced in significant volumes at reasonable cost from sustainable domestic sources of biomass and waste material. The Co-Optima researchers' approach reduced the need for time-consuming experimental determination of properties, increasing the number of blendstocks that could be examined.

MAJOR ANALYSIS FINDINGS AND IMPACTS

Cost-Competitive Fuels with Low GHG Emissions

Demonstrated potential to deliver new low-carbon fuels at prices competitive with those of conventional fuels:

- Identified LD fuels with modeled minimum fuel selling prices (MFSPs) from \$2.50–\$4/GGE.
- Identified MD and HD fuels with modeled MFSPs ≤\$4/GGE.

Reductions in Operating Costs

Identified other savings related to HD vehicle operation:

- Decreased the need for HD fuel aftertreatment, reducing lifetime operating costs.

Value to Refiners

Quantified potential value of bioblendstocks to refiners:

- Determined how changes in key fuel properties such as RON, S, sulfur content, and CN could increase potential profitability.
- Estimated a breakeven value of proposed blendstocks as high as \$110/barrel of oil equivalent.

The top bioblendstock candidates for light-duty (LD), medium-duty (MD), and heavy-duty (HD) vehicles were identified based not only on their ability to reduce GHG emissions by at least 50% (for turbocharged spark ignition) or 60% (for all other combustion approaches), but also on whether fuel prices could be competitive with those of conventional fuels. These shortlisted candidates included blendstocks produced from corn stover, woody biomass, and used cooking oil, which show potential to be produced at commercial scale and deliver prices at the pump below \$4 per gasoline gallon equivalent (GGE).

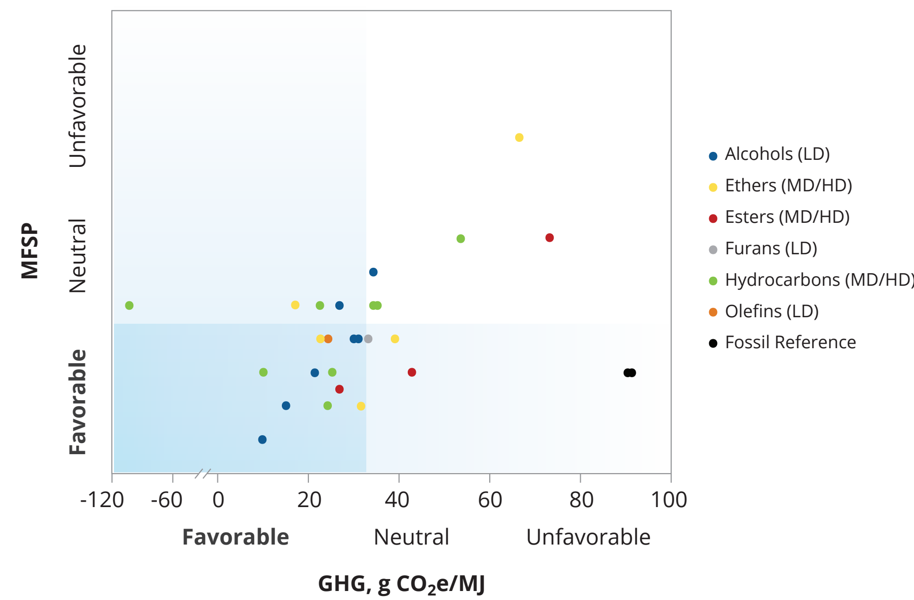
Predicting Longer-Term Impacts with Benefits Analyses

When these new fuel-engine combinations make it onto U.S. highways, what changes can be expected? Researchers used macroeconomic, system dynamics, and consumer choice models, many of which were developed specifically for the Co-Optima initiative, to analyze potential broader industry economic and environmental benefits.

Analysts linked these sophisticated models to explore wide-ranging scenarios for vehicle sales, biofuel production, and job growth, as well as environmental impacts. The results projected how fuel economy improvements, emissions reductions, and other factors might interplay with the cost of new technologies and fuels to impact market demand for new vehicles and fuels, as well as potential domestic job growth through the construction and operation of production facilities.

Evaluations revealed the potential for the candidate bioblendstocks—especially those with synergistic blending properties—to add value for petroleum refining operations. Researchers project that the breakeven value of proposed blendstocks could be as valuable as $110 per barrel of oil equivalent. The blendstocks also have the potential to decrease HD engine aftertreatment, reducing lifetime operating costs and improving compliance with strict emissions requirements.

Top Blendstock Candidates Demonstrate Beneficial Price and Emissions Trade-Offs



Top bioblendstocks deliver low emissions at a cost-competitive price.

Photo: iStock

WHAT'S NEXT

The Bridge to Net-Zero-Carbon Emissions

Photos: Getty Images

Accelerating Opportunities in a Changing World

What else needs to happen before Co-Optima knowledge and technical results can meaningfully impact the marketplace and the environment? These changes can only occur if producers and manufacturers undertake further development, scale-up, and deployment of the low-carbon fuels and efficient engine technologies that were discovered through this initiative. Ongoing support from national laboratory and university researchers, as well as policies aimed at accelerating decarbonization, will be vital to the success of any commercialization efforts.

The context for new fuels and vehicle technologies has changed significantly since the Co-Optima initiative kicked off 6 years ago. Climate change is accelerating, increasing the urgency to drastically reduce the greenhouse gas (GHG) emissions responsible for global warming. Strategies for U.S. energy decarbonization must factor in decisions about all transportation modes—including land, air, rail, and marine—to meet ambitious targets for addressing this threat.

POTENTIAL FUTURE CO-OPTIMA-ENABLED TRANSPORTATION ADVANCES

Future research has the potential to expand on Co-Optima findings with:

- Commercial deployment of net-zero-GHG technologies for hard-to-electrify transportation modes.
- Clean and efficient fuel and combustion options for on-road transport prior to broader EV deployment.
- Fuel property-based methods to identify the most advantageous combustion approaches used in hard-to-electrify sectors.
- Efficient biomass and waste utilization to produce sustainable fuels with performance advantages.
- Reduced costs of emissions compliance and lower impact on local air quality.
- Affordable, convenient, and efficient mobility solutions for people and goods across all economic and social groups.

Automakers plan to dramatically expand production of on-road electric vehicles (EVs) in the near future. EVs and plug-in hybrid EVs (PHEVs) offer low source-to-wheel GHG emissions when the electricity used to charge them is generated from clean renewable sources. PHEVs combined with low-net-carbon-emissions or net-zero-carbon-emissions fuels such as those identified by Co-Optima provide both short- and long-term solutions to reducing transportation emissions.

At the same time, the choice of a propulsion system will always depend on how a vehicle is being used. Even with an expected steep increase in passenger vehicle electrification in the coming years, internal combustion engines will continue to be used in the United States for decades. Big heavy vehicles, such as long-haul freight trucks and off-road equipment, will still require powerful diesel engines to haul large loads of cargo hundreds of miles across varied terrain or operate away from the electric grid.

EV adoption will be more gradual in countries where fleet turnover is much slower than in the United States. In the meantime, the combination of sustainable liquid fuels uncovered by Co-Optima research with engines for hybrid electric vehicles can reduce the carbon and other pollutant emissions of vehicles now, while enabling a faster transition to a net-zero-carbon-emissions transportation future.

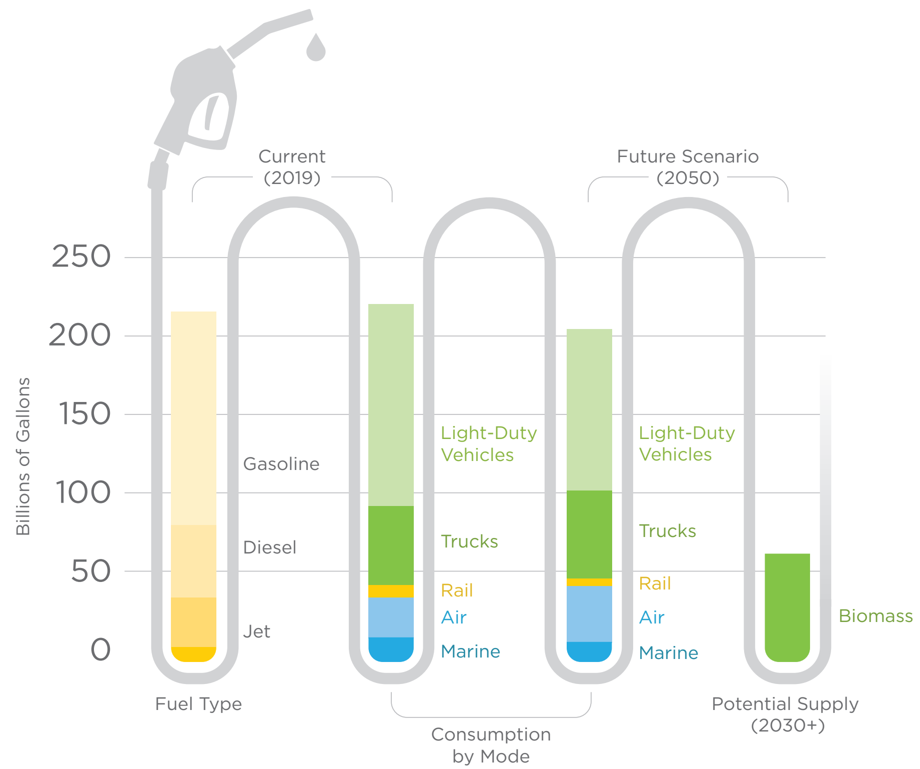
Building Momentum in Air and Marine Transportation

Airplanes and cargo ships are likely to use approximately 70% of available low-net-carbon-emissions fuels as electrification of cars and smaller trucks becomes more widespread and decreases liquid fuel demand for on-road transportation. These off-road transportation modes have different fueling requirements, from airplanes' stringent safety regulations to ships' huge cargo loads and lengthy periods between refueling.

Co-Optima breakthroughs in chemical structure-fuel property relationships, property predictions, advanced simulations, techno-economic and life cycle analyses, and other areas are already contributing to the development of sustainable fuels for these transportation modes. Studies show that biomass could eventually meet 100% of future demand for air, marine, and rail fuel, while still leaving a supply of feedstock to produce fuel for some on-road vehicles.

New knowledge and pollution-reducing fuels and engine technologies developed by Co-Optima researchers for use in on-road heavy-duty vehicles may also help reduce pollution from marine, rail, off-road, and airplane engines. The improved understanding of chemical structure and fuel property impacts on soot formation offers a roadmap to similar approaches for these other transportation modes. Together, these advances will accelerate the decarbonization of transportation on the land, in the air, and across the water.

Sustainable Fuel Use Will Shift to Hard-to-Electrify Sectors



Feedstock supply is projected to meet sustainable fuel production demand for some hard-to-electrify sectors including marine, jet, and rail, as well as part of the heavy-duty on-road transportation sector. Source: AEO

Tapping into a Potential 60-Billion-Gallon Fuel Supply

Is there enough sustainable biofuel to meet a significant fraction of future on-road transportation needs? Most likely there is—with the right investments in production and conversion technologies.

The Bioenergy Technologies Office's Billion-Ton Study identified the potential to convert 1 billion tons of sustainable domestic waste and biomass feedstocks into 60 billion gallons of fuel per year. These include sources such as forestry and agricultural byproducts, algae, discarded cooking oil, and even manure.

While Co-Optima research focused on fuel blends containing up to 30% bio-based or waste-based content, this foundational knowledge can also be applied to higher blend levels or fuels made from electricity and carbon dioxide (so-called e-fuels). Decarbonizing the on-road transportation system will require at least 90% levels of sustainable fuel content, with an eventual shift to 100% net-zero-carbon-emissions fuels.

Ultimately, expanded commercial production of sustainable and affordable biofuels will be required to meet liquid fuel demands. As the primary demand for liquid fuels shifts from light-duty vehicles to heavy-duty trucks, planes, and cargo vessels, the supply of ethanol currently used in cars will be available for conversion to fuels suitable for other applications.

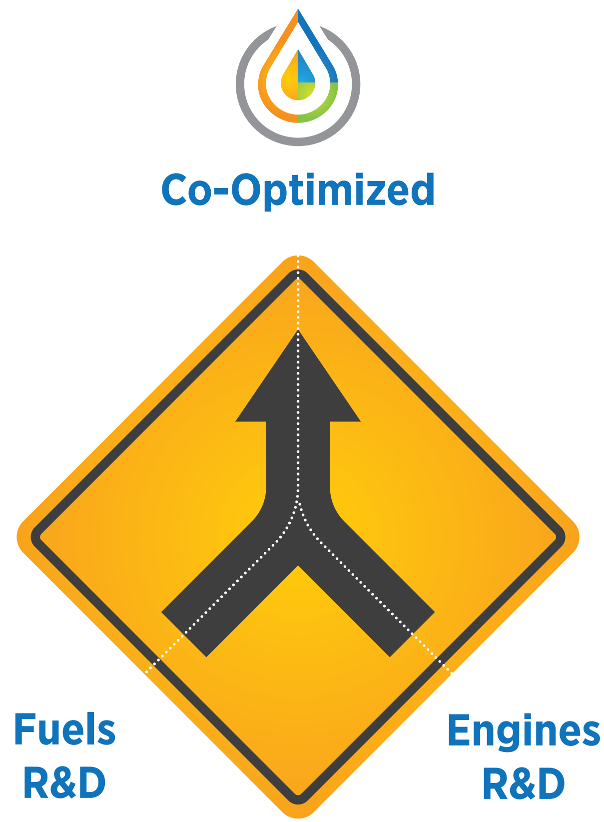
Additional research is required to ensure these low-carbon, zero-carbon, and even net-negative-carbon-emissions fuels are fit for their intended purpose. Standards need to be established for these new fuels, especially for high-level blends and 100% biofuels with properties that differ greatly from those of today's fuels.

Establishing New Engine Parameters to Optimize Use with New Fuels

Building on Co-Optima results and fully optimizing engines for use with fuels that contain high levels of bioblendstocks or fuels that are 100% bio-based will require additional R&D. Research by manufacturers is essential to determine what more significant changes in engine operation and component materials will be needed to approve use of these sustainable fuels in commercial engines.

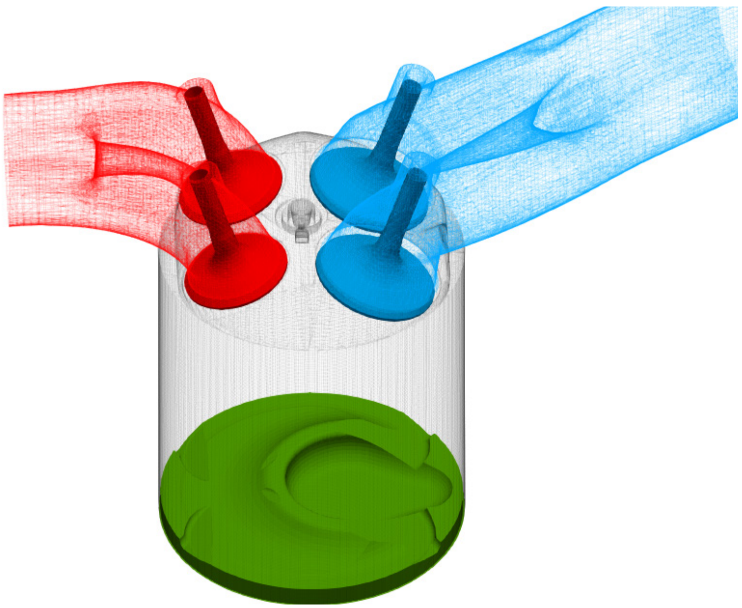
This research could result in new engine modifications beyond those contemplated by Co-Optima researchers, extending the efforts to enable or exploit different fuel properties for lower costs, lower emissions, and higher efficiency. Reducing criteria pollutant and GHG emissions will also help more equitably distribute these environmental benefits, diminishing the concentration of poor air quality near highways and transportation hubs that are frequently located in proximity to underserved populations and helping limit the impact of climate change on vulnerable communities.

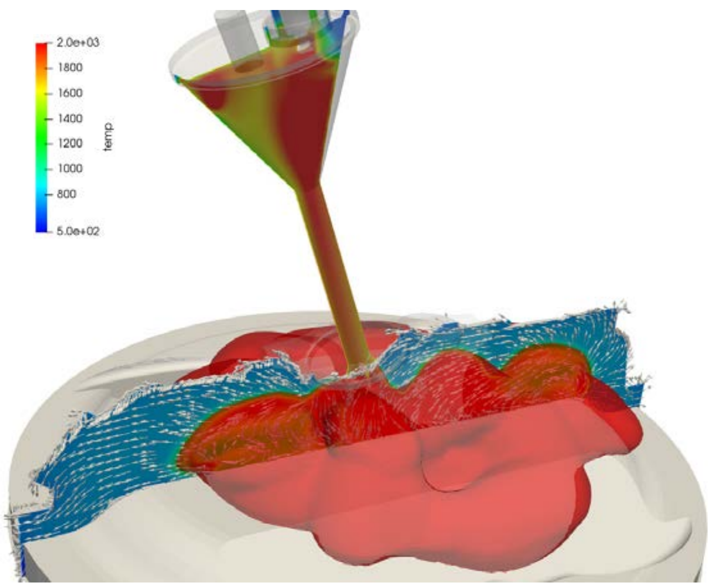
Ultimately, these new fuels and engines identified through Co-Optima research will burn cleaner, produce fewer life cycle GHG emissions, and make important contributions to the nation's transition to a net-zero-carbon-emissions energy future.



TOOLS AND DATA

Speeding Up Evaluations, Increasing Accuracy, and Expanding Access





Figures: ANL

High-Level Computational Tools

Fuel blend performance can be evaluated much faster using simulations, rather than testing in actual engines. The Co-Optima team developed a wide range of robust, validated tools to capture fuel-engine interactions with greater accuracy, improve the efficacy of predictions, and reduce computation time. The fast solvers, lower-order models, and algorithms make it possible to evaluate an unprecedented number of fuel blends in days rather than months.

These new tools include high-fidelity computational fluid dynamics (CFD) simulations and lower-order models that leverage acceleration techniques based on high-performance computing and machine learning. New approaches make it possible for the engine industry to plug routinely used commercial codes into the models. These methods can be adapted for other modes of transportation, ensuring these Co-Optima computational tools will help increase the rate of innovation for years to come.

These innovative Co-Optima tools and models include:

- **Fuel property prediction tools and models** – To estimate a range of physical, chemical, and combustion fuel properties.
- **Multiphase in-nozzle flow and spray models** – For fuel blends for both spark- and compression-ignition engine simulations.
- **Turbulent combustion models** – For a wide range of combustion regimes.
- **Chemical kinetic tools** – To accelerate fuel property prediction with faster calculations of laminar flame speed, ignition delay, octane numbers, and other properties.
- **Lower-order models of fuel and engine performance models** – Trained using simulations and experimental data to predict fuel-engine co-optimization performance.
- **Gaussian process optimization algorithm** – To identify subsets of blend candidates for engine simulations.

These tools were rigorously validated using optical and metal engine platforms with many fuels at several national laboratories.

>60 new kinetic mechanisms

>10,000 downloads from the Fuel Properties Database

14 combustion turbulence and multiphase flow models

7 CFD models integrated into commercial software

Publicly Available Tools and Data

Co-Optima researchers developed publicly available data repositories, numerical algorithms, and computational tools. The following data and tools can be accessed online by the wider research community: www.energy.gov/fuel-engine-co-optimization/co-optima-tools-and-data.

ALFABET

bde.ml.nrel.gov/

ALFABET (A machine-Learning derived, Fast, Accurate Bond dissociation Enthalpy Tool) allows researchers to identify the most promising fuels for lower emissions and greater engine efficiency in seconds rather than days. This online tool predicts bond dissociation energies of organic molecules and produces high-quality estimates of the strength of organic bonds. For fuels, weak bonds often determine initial reactions in combustion chemistry, influencing autoignition and soot formation.

Co-Optimizer Tool

github.com/NREL/cooptima-co-optimizer

The Co-Optimizer tool makes it possible to assess trade-offs involving complex variables such as production scale and economics, life cycle emissions, and infrastructure compatibility for new blendstocks. After identifying blendstocks with the properties needed to maximize turbocharged spark-ignition engine efficiency when blended into petroleum base fuels, researchers use the tool's models to identify fully blended fuels that meet fuel-quality specifications, and then compare a smaller subset across a wide range of market introduction scenarios.

ECNet Tool

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 available. This software reduces the time required to construct models while increasing model accuracy.

Fuel Properties Database

www.nrel.gov/transportation/fuels-properties-database

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

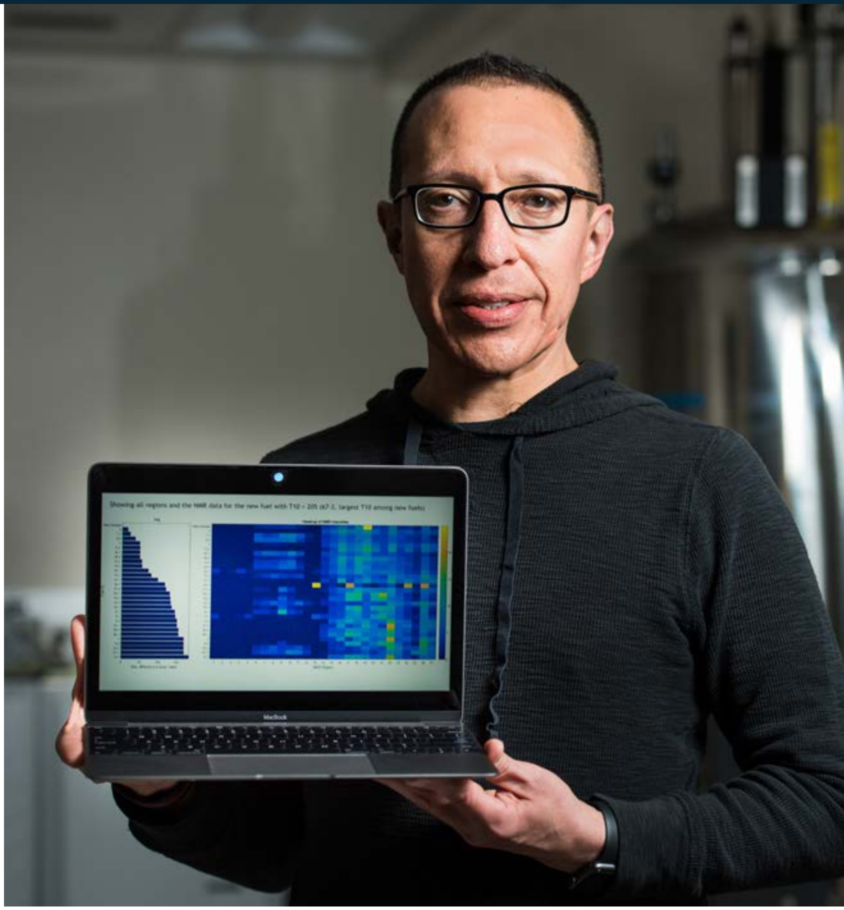


Photo: PNNL

RetSynth Tool

github.com/sandialabs/RetSynth

The RetSynth (retrosynthesis) tool can be used to rapidly identify and evaluate the viability of pathways for producing bio-based molecules of interest in blendstock development. 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 genes, reaction conditions, and theoretical yields for the target molecule. It can also rank optimal biological pathways with the smallest number of steps.

Yield Sooting Index Tool

ysi.ml.nrel.gov/

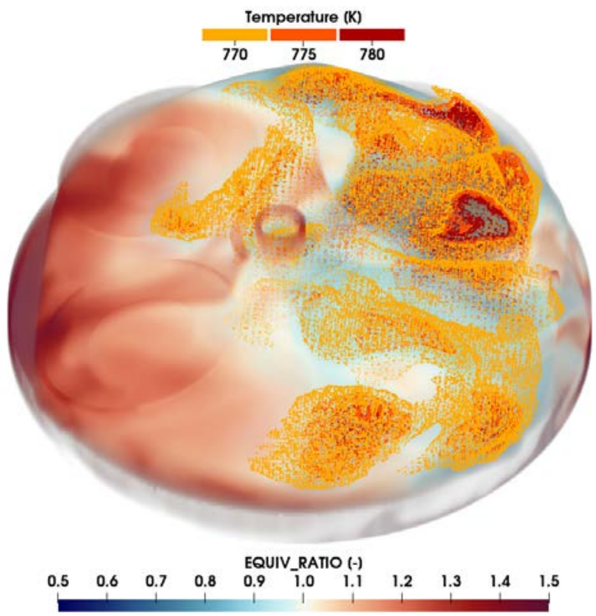
Researchers integrated the YSI computational method into a tool that rapidly estimates the sooting tendency of fuel blendstocks, allowing the interactive development of potential new blendstocks that meet YSI targets. Expanding the breadth of experimental data on sooting tendency in this database improved the accuracy of soot production predictions.

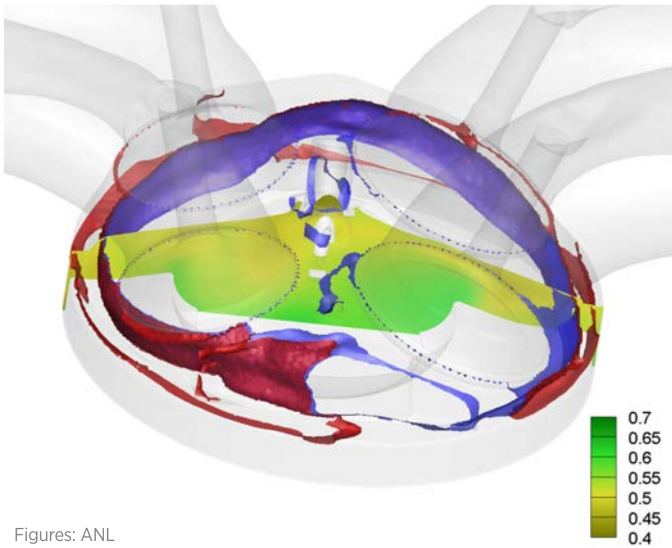
Zero-RK Tool

github.com/LLNL/zero-rk (Zero-RK tool)

combustiontools.llnl.gov (models based on Zero-RK)

Zero-RK (zero-order reaction kinetics) software reduces the time required to simulate chemically reacting systems by orders of magnitude, while delivering accurate results. The tool's sparse, preconditioned, adaptive matrix methods are applied to a number of canonical reaction models that can be used to simulate detailed fuel chemistry for internal combustion engines (ICEs), calculate reaction network sensitivities, and debug problematic mechanism definitions. These models include constant-volume and constant-pressure reactors, variable-volume reactors (e.g., rapid compression machines, ICEs), perfectly stirred reactors, and laminar premixed and diffusion flames.





Figures: ANL

Sharing Findings with Key Audiences

High-Impact Publications

Getting the word out on approaches, results, and tools was a critical first step in providing industry and other key stakeholders with the scientific underpinnings needed to build on Co-Optima research. Researchers established a strong scientific publication track record over the 6 years of the initiative.

Journal articles, conference papers, technical reports, and other research publications spanned topics including light-duty (LD), medium-duty (MD), and heavy-duty (HD) applications; blendstock structure-property relationships; emissions; new software tools; and techno-economic and life cycle analyses. Outreach publications, including fact sheets and annual Year in Review reports, communicated goals, progress, and top-level findings to a broader audience.

The high-impact publications below provide just 4 examples illustrating the breadth and depth of Co-Optima research and development.

>250 total publications

>2,500 publication downloads

>200 journal articles

>50 conference papers

14 technical papers


Progress in Energy and Combustion Science

What fuel properties enable higher thermal efficiency in spark-ignited engines?

Co-Optima research demonstrated how 6 fuel properties—research octane number, octane sensitivity, latent heat of vaporization, laminar flame speed, particulate matter index, and catalyst light-off temperature—impact the potential of bioblendstocks to enable high thermal efficiency in boosted spark-ignition (SI) engines for LD vehicles.
doi.org/10.1016/j.pecs.2020.100876

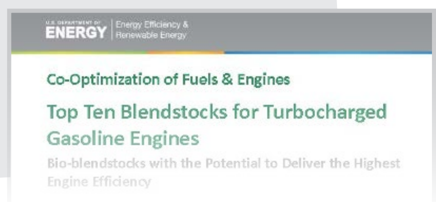

Energy & Environmental Science

ROYAL SOCIETY OF CHEMISTRY

ANALYSIS

Energy, economic, and environmental benefits assessment of co-optimized engines and bio-blendstocks

Researchers modeled deployment of LD engines co-optimized with 3 biofuel blends to deliver 10% higher engine efficiency, quantifying potential effects on U.S. petroleum consumption, greenhouse gas (GHG) emissions, particulate matter emissions, water consumption, and jobs.
doi.org/10.1039/D0EE00716A

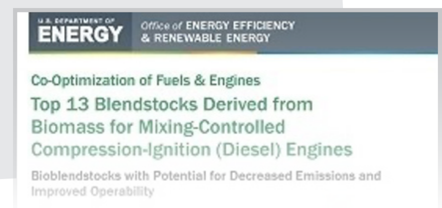

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Co-Optimization of Fuels & Engines

Top Ten Blendstocks for Turbocharged Gasoline Engines

Bio-blendstocks with the Potential to Deliver the Highest Engine Efficiency

Researchers identified 10 performance-advantaged LD boosted SI biofuel blendstock candidates with properties capable of delivering fuel economy gains as high as 10%.
doi.org/10.2172/1567705


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

Co-Optimization of Fuels & Engines

Top 13 Blendstocks Derived from Biomass for Mixing-Controlled Compression-Ignition (Diesel) Engines

Bioblendstocks with Potential for Decreased Emissions and Improved Operability

Researchers identified 13 biofuel blendstock candidates with the potential to be produced at a competitive cost and reduce GHG emissions by at least 60% when used in MD and HD mixing-controlled compression-ignition engines.
doi.org/10.2172/1806564

For more detailed information on other Co-Optima publications, visit the website: www.energy.gov/fuel-engine-co-optimization/co-optima-publications.

Other Communications Outreach

>650 webinar attendees

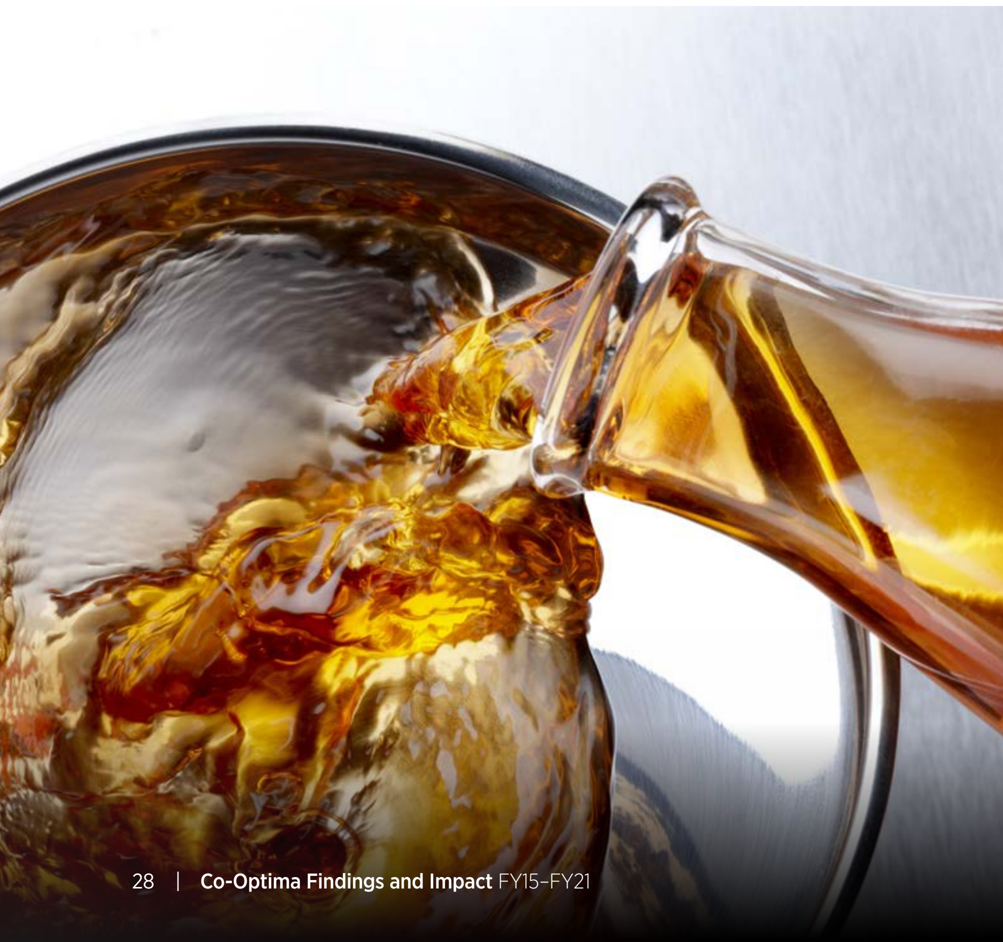
>27 online news items and press releases

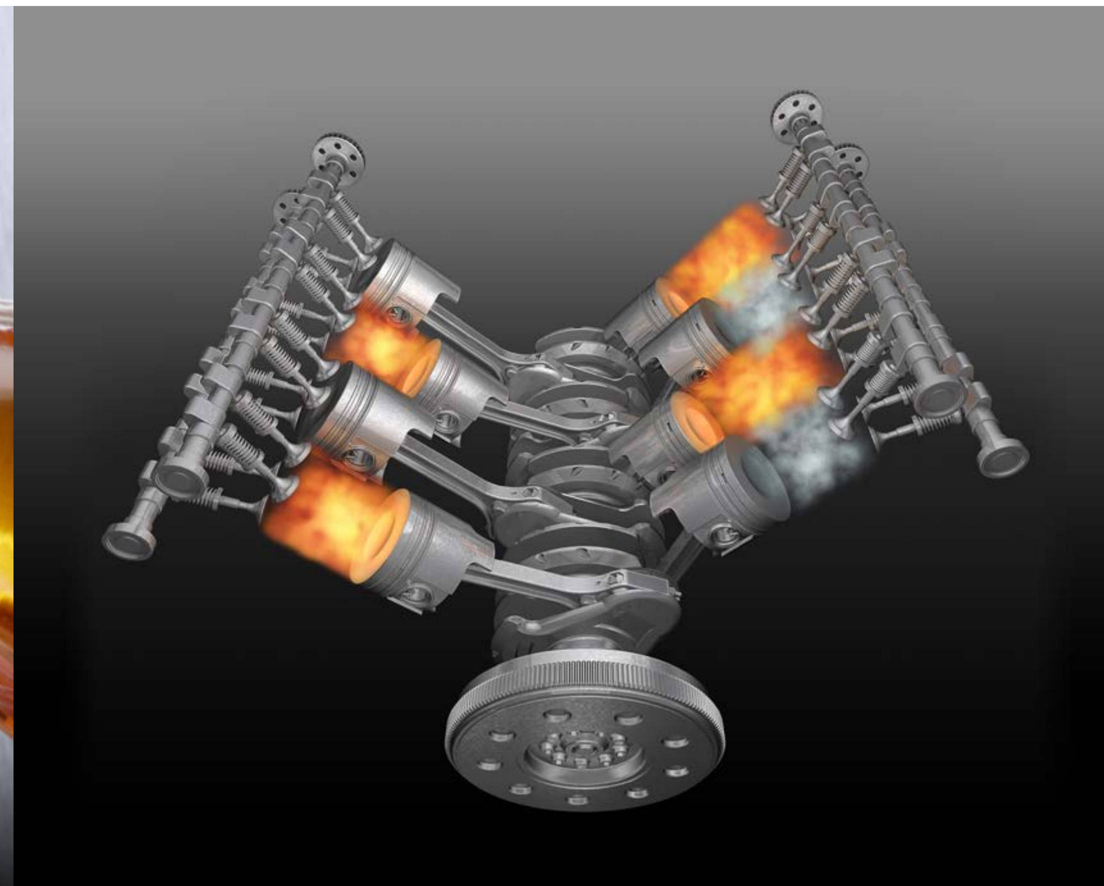
>190 media stories and mentions

Beyond publications, information on research activities and accomplishments was shared via webinars, the Co-Optima website, online news items, press releases, social media, and other promotional efforts. This outreach expanded awareness of the initiative in the research community, across industry, and with other immediate Co-Optima stakeholders, as well as with the general public. These communications also led to coverage by numerous digital and traditional media outlets.

For more information on Co-Optima news stories, press releases, webinars, and more, visit the website: www.energy.gov/fuel-engine-co-optimization/co-optima-news.

Photos: iStock



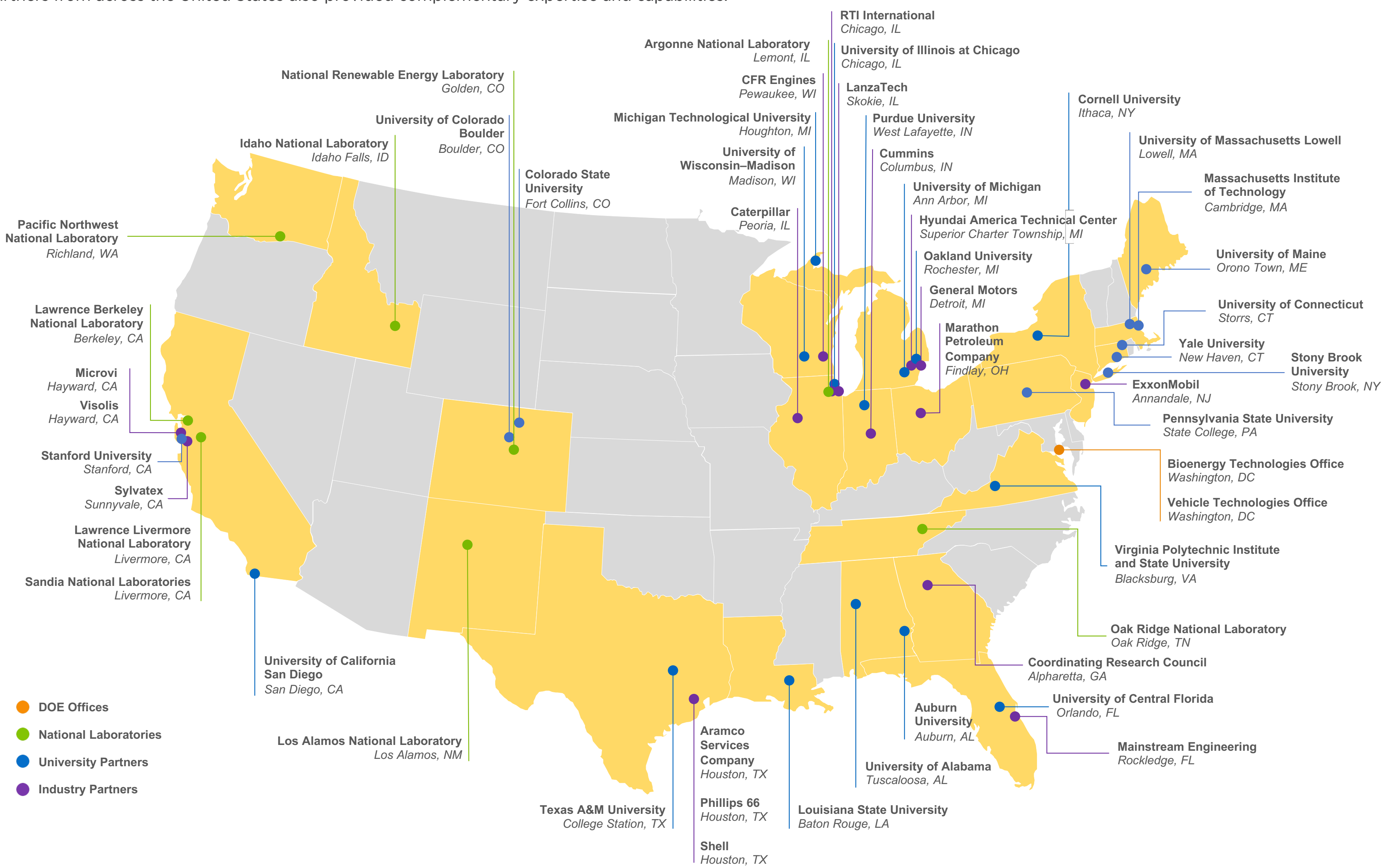


PARTNERS AND STAKEHOLDERS

Collaboration Vital to Setting Priorities and Meeting Goals

DOE, National Laboratory, University, and Industry Research Partners

Collaboration was vital to success of the Co-Optima initiative. Not only did joint sponsorship by the Office of Energy Efficiency and Renewable Energy's (EERE's) Vehicle Technologies Office (VTO) and Bioenergy Technologies Office (BETO) connect researcher from different fields and backgrounds at 9 national laboratories, but numerous university and industry partners from across the United States also provided complementary expertise and capabilities.



From the start, additional stakeholders were crucial in helping to define Co-Optima needs and priorities. Engaging external stakeholders from U.S. and international fuel and vehicle industries, government agencies, and research institutions helped the Co-Optima initiative better gauge potential research directions and market viability of potential innovations.

Stakeholders and the research team met at "listening day" events, trade association conferences, one-on-one stakeholder meetings, monthly presentations of technical highlights, DOE review meetings, and other forums. The Co-Optima leadership team also engaged with an external advisory board consisting of industry, university, and regulatory leaders several times each year.

To increase near-term commercial impact in the final years of the initiative, DOE provided opportunities for stakeholders to work directly with Co-Optima national laboratory partners on R&D most relevant to industry aims. These industry-led projects, many of which are ongoing, were selected by competitive processes and engaged the national laboratories' unique experimental and computational capabilities. The industry partners contributed a market-facing perspective, specific complementary expertise, and cost sharing to address key research barriers at the fuel-engine interface.

Co-Optima Leadership Team

Current Members

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Pacific Northwest National Laboratory

Anthe George
Sandia National Laboratories

Robert McCormick
National Renewable Energy Laboratory

Robert Wagner
Oak Ridge National Laboratory

Prior Members

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John Holladay
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Sandia National Laboratories

Art Pontau and Paul Bryan
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Laboratory photos courtesy of:

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Lawrence Berkeley National Laboratory (LBNL)
Los Alamos National Laboratory (LANL)
National Renewable Energy Laboratory (NREL)
Oak Ridge National Laboratory (ORNL)
Pacific Northwest National Laboratory (PNNL)
Sandia National Laboratories (SNL)

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