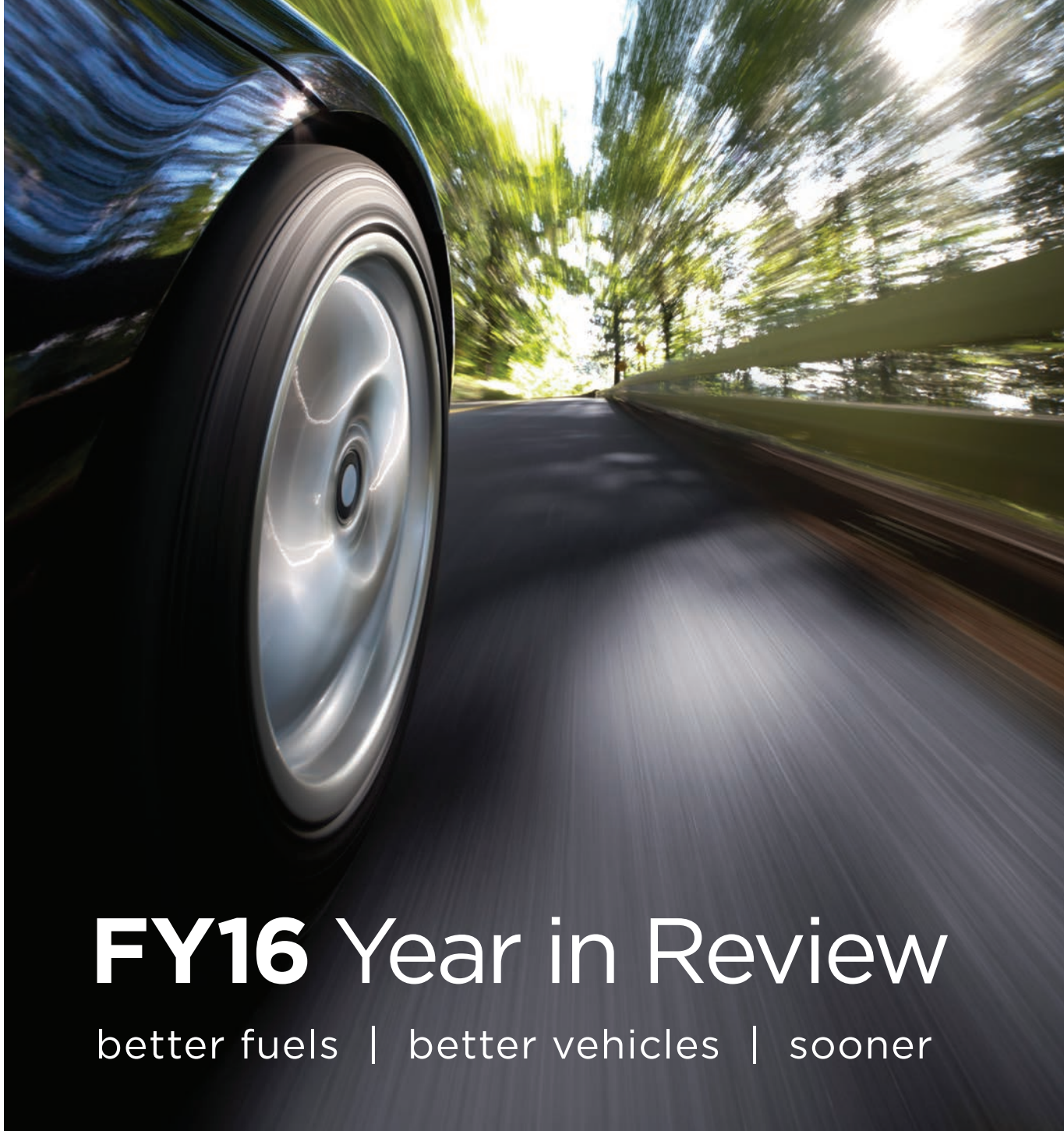
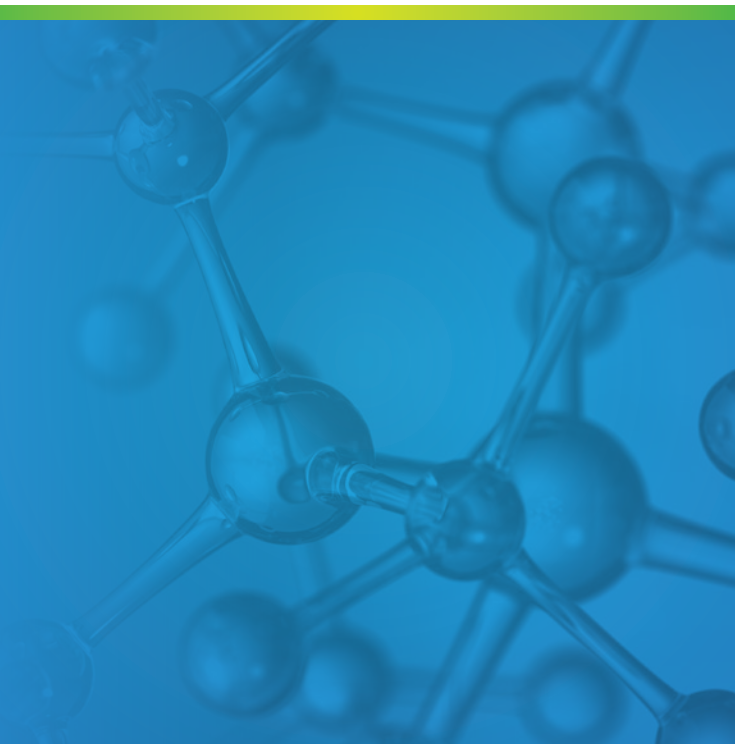




Co-Optimization of Fuels & Engines



FY16 Year in Review

better fuels | better vehicles | sooner

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

Transportation accounts for 70% of U.S. petroleum consumption and 27% of the country's greenhouse gas (GHG) emissions, and the internal combustion engines (ICEs) that generate most of these emissions will continue to power vehicles for decades to come. The U.S. Department of Energy's (DOE's) Co-Optima initiative is accelerating the introduction of affordable, scalable, and sustainable fuels and high-efficiency, low-emission engines with a first-of-its-kind effort to simultaneously tackle fuel and engine research and development (R&D).

Co-Optima is conducting research to identify the fuel properties and engine design characteristics needed to maximize vehicle performance and affordability, while deeply cutting harmful emissions. Rather than endorsing a single solution, this initiative is designed to arm industry, policymakers, and other key stakeholders with the scientific foundation and market intelligence required to make investment decisions, break down barriers to commercialization, and bring new high-performance fuels and advanced engine systems to market sooner.

DOE's Office of Energy Efficiency & Renewable Energy (EERE) has brought together nine national laboratories—the National Renewable Energy Laboratory and Argonne, Idaho, Lawrence Berkeley, Lawrence Livermore, Los Alamos, Oak Ridge, Pacific Northwest, and Sandia National Laboratories—to collaborate on this groundbreaking research. The outcome of this effort will be new tools, data, and knowledge to pave the way for future generations of fuel and vehicle innovations.

Letter from the Leadership Team

In its first year, the Co-Optima initiative moved from robust concept to concrete results. The two DOE offices, nine national laboratories, and industry stakeholders that compose Co-Optima successfully worked to integrate fuels and engine R&D, breakdown barriers, and tackle challenges. This report highlights the progress made by Co-Optima in fiscal year 2016.

In this inaugural year, our parallel Co-Optima research tracks have focused on fuels and engine technologies related to spark-ignition (SI) and advanced compression ignition (ACI) systems. The first phase, Thrust I, has concentrated on:

- ▶ Improving near-term SI engine efficiency
- ▶ Assessing desirable properties for bio-derived or bio-based components (blendstocks) to be blended with petroleum-derived gasoline
- ▶ Identifying more than 40 promising blendstock candidates
- ▶ Evaluating the impact of discrete fuel properties on advanced SI engine performance.

Researchers have also initiated R&D on Thrust II ACI combustion strategies focused on achieving higher efficiency with lower levels of harmful emissions than can be achieved today. We evaluated fuel property impacts on kinetically controlled and low-temperature combustion (LTC) strategies and began to improve our understanding of how co-optimized fuel properties and engine strategies can contribute to longer-term solutions.

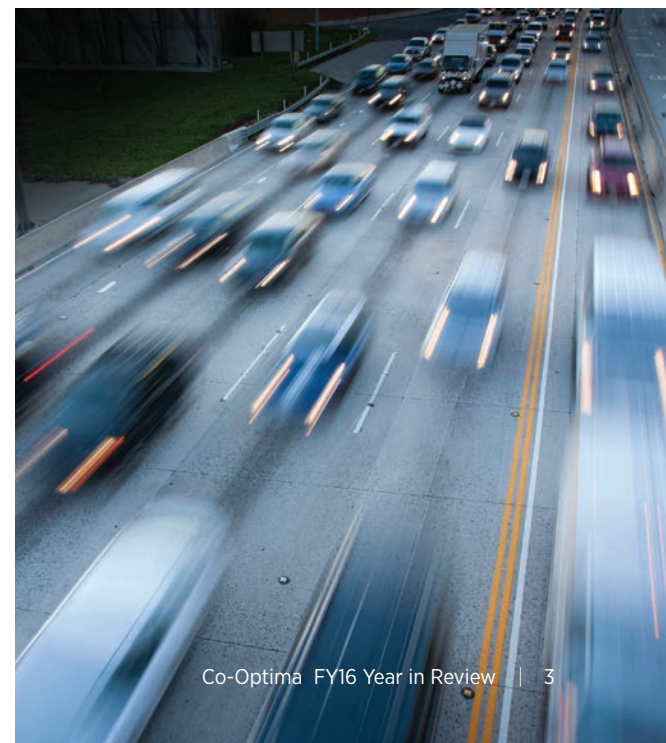
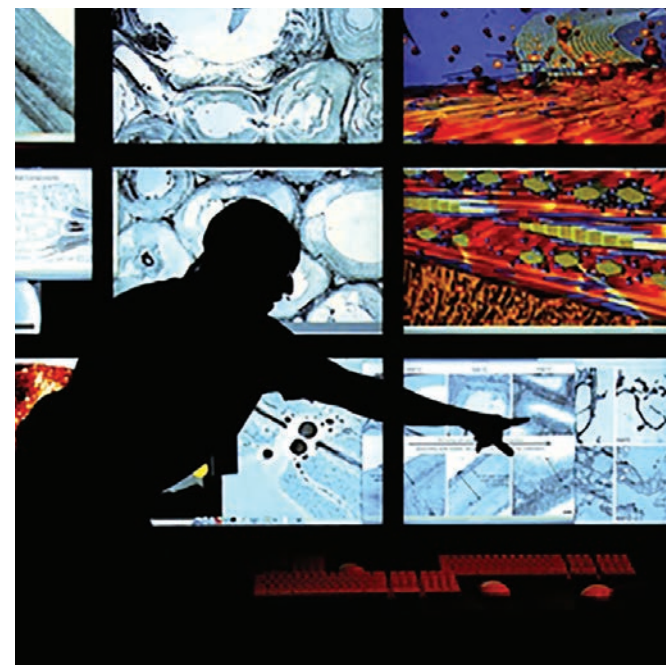
Not only is Co-Optima integrating fuel and engine research efforts, but we're addressing deployment barriers and fostering technological innovation. Co-Optima is also facilitating research collaboration by bringing together some of the nation's top fuel and engine scientists, engineers, and analysts. With the support of EERE's Vehicle Technologies and Bioenergy Technologies Offices, we are pursuing a technology-neutral approach. At the same time, ongoing dialogue with a wide range of stakeholders ensures that our team is guided by marketplace realities and driven to develop technology solutions that will substantially lower market barriers.

We're encouraged by initial evaluations that indicate technologies and strategies under exploration by Co-Optima researchers will have the potential for significant passenger vehicle fuel economy improvements. As Thrust I and Thrust II research progresses, our goal—better fuels, better vehicles, sooner—is within reach.

John Farrell
National Renewable Energy
Laboratory

John Holladay
Pacific Northwest National
Laboratory

Robert Wagner
Oak Ridge National
Laboratory



Big-Picture Targets

Co-Optima's ultimate goal is to provide U.S. industry with the R&D needed to strengthen energy security and stimulate economic growth while reducing harmful emissions from transportation.

Deliver

\$30-\$40 BILLION IN
COST SAVINGS
annually via improved fuel economy

INCREASE ENERGY INDEPENDENCE with
biofuels from domestic feedstocks supplying as much as
15% OF LIQUID FUELS BY 2035

Spur the **U.S. ECONOMIC GROWTH**
with the establishment of

500,000 NEW JOBS

Accelerate the **SPEED OF DEPLOYMENT**
with commercial introduction of **NEW FUELS/
TECHNOLOGIES BY 2025**

Contribute to national goal of
80% REDUCTION in transportation
GHG EMISSIONS by 2050

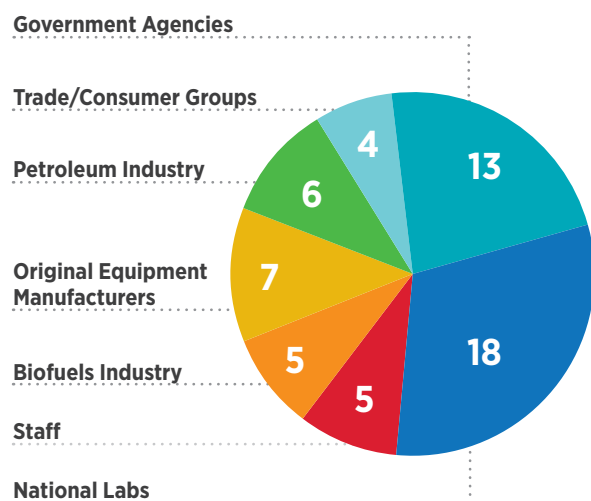
Improve passenger vehicle
FUEL ECONOMY BY
50% 15% beyond the projected
results of existing R&D efforts

Dialogue with Stakeholders

To help ensure the success of this ambitious initiative, Co-Optima leaders have established ongoing dialogue with government and industry decision makers — through “listening day” events and outreach to trade associations and other organizations. Representatives from stakeholder groups have been invited to weigh in on key research components and priorities, and Co-Optima has built and relies on an external advisory board.

Stakeholders have emphasized the importance of identifying concrete value propositions, clearly defining project scope, taking an inclusive approach across agencies and levels of government,

Listening Day Workshop Participation Number of Attendees per Sector



and establishing collaborative dialogue. Because of these conversations, Co-Optima is pairing R&D efforts with exploration of market realities. This dialogue has made it possible to identify research needs, potential risks, and mitigation strategies in the areas of engine efficiency and performance, fuel production and distribution, infrastructure compatibility, and retail sales.

Particularly valuable perspectives have been provided by stakeholders on overall market viability, considering the impact of factors including economic conditions, investment requirements, deployment timelines, government policy, and consumer acceptance in their assessment of how to best cultivate marketplace acceptance.

The national labs and EERE recognize that continued exchanges with these partners will be critical at each stage of the Co-Optima initiative, and plans are already underway to build on this foundation of stakeholder engagement. Additional listening day and stakeholder events are being scheduled.

A Funding Opportunity Announcement (FOA) was released in FY16 to involve universities in Co-Optima research, and it is anticipated that awards will be announced in the first half of 2017.

Key Listening Day Takeaways

Topic	Stakeholder Observations
Scoping New Horizons for Fuels and Vehicles	<ul style="list-style-type: none"> New fuels have to be drop-in compatible with existing distribution equipment and vehicles to avert costs and complexities of major infrastructure changes.
Spark Ignition Applications	<ul style="list-style-type: none"> Successful co-optimization will rely on market certainty, as well as on engine and fuel producer cooperation. It will be important to explore options other than octane, compression ratios, and clean LTC.
Advanced Combustion Applications	<ul style="list-style-type: none"> There is no low-GHG fuel substitute commercially available at the needed volumes. An optimized system of fuels/engines might prove more tractable by blending fuels.
Barriers to Deployment	<ul style="list-style-type: none"> The best approach to overcoming barriers combines policy with successful technology implementation, incentives, consumer outreach, and infrastructure compatibility.
Stakeholder Engagement	<ul style="list-style-type: none"> Buy-in from and market readiness of all stakeholders will be vital to successful deployment of new fuels and engines. Representation from consumer groups should be expanded.

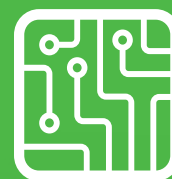
Integrated Capabilities in Support of End-to-End Scope

Co-Optima's integrated approach merges the previously independent areas of low-carbon fuel and combustion R&D, spanning a diverse range of capabilities and expertise. The initiative's end-to-end scope ranges from basic science research to analysis of deployment factors. Activities that often cut across the key research areas are outlined below.



High-Performance Fuels

- ▶ Identify promising bio-derived blendstocks
- ▶ Develop selection criteria for fuel molecules
- ▶ Identify viable production pathways



Modeling and Simulation Toolkit

- ▶ Leverage high-fidelity simulation capabilities
- ▶ Extend the range, confidence, and applicability of engine experiments

Advanced Engine Development

- ▶ Quantify interactions between fuel properties, engine design, and operating strategies
- ▶ Enable optimal design of efficient, emission-compliant engines



Analysis of Sustainability, Scale, Economics, Risk, and Trade

- ▶ Analyze energy, economic, and environmental benefits to the United States
- ▶ Examine routes to feedstock production at scale through existing biomass markets



Fuel Properties

- ▶ Identify critical properties and allowable ranges
- ▶ Systematically catalog properties
- ▶ Predict fuel blending behavior

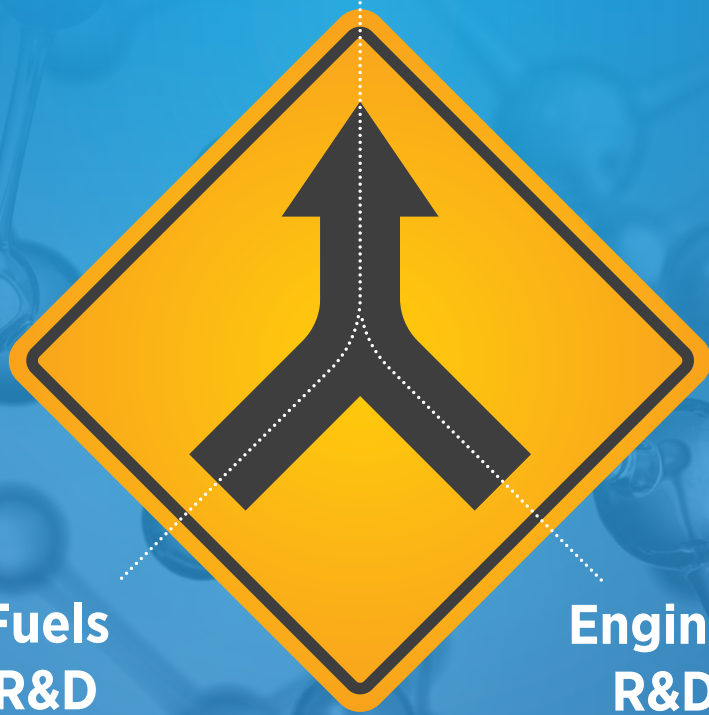


Market Transformation

- ▶ Identify and mitigate challenges of moving new fuels and engines to market
- ▶ Engage with full range of stakeholders



Co-Optimized



Fuels
R&D

Engines
R&D



Using the Past to Guide Future Success

A detailed examination of previous fuel and vehicle introductions and input from stakeholders are providing the Co-Optima team with key insights to guide the direction of the R&D toward the successful deployment of new technologies. A thorough review of existing research is exploring the potential impact of vehicle distribution patterns, infrastructure compatibility, feedstock supply, and laws and incentives. For example, the high volume of cellulosic biomass makes storage and transportation expensive, but previous studies show that processing these sustainable, domestically produced feedstocks into pellets can make shipping and warehousing efficient.

This extensive review of existing research also confirmed that compatibility with current infrastructure, extensive consumer outreach, and consistent government policies will be vital to the success of any new fuel and engine introductions. Identification of these possible market barriers and mitigation strategies will help industry and government decision makers reduce risks involved in eventual commercialization.



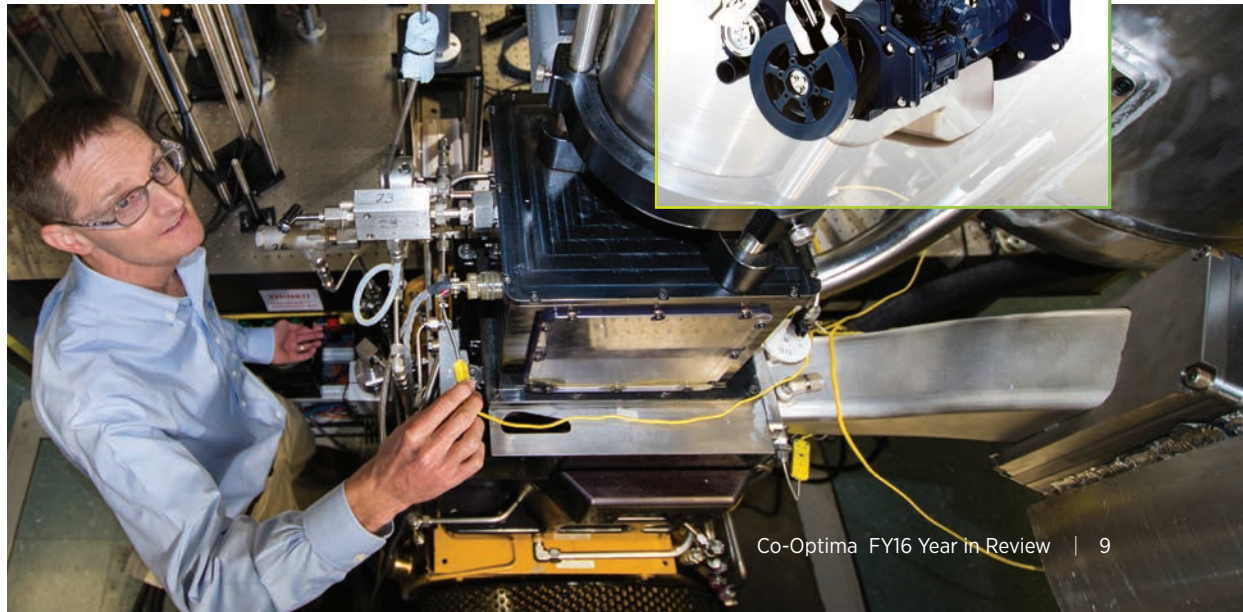
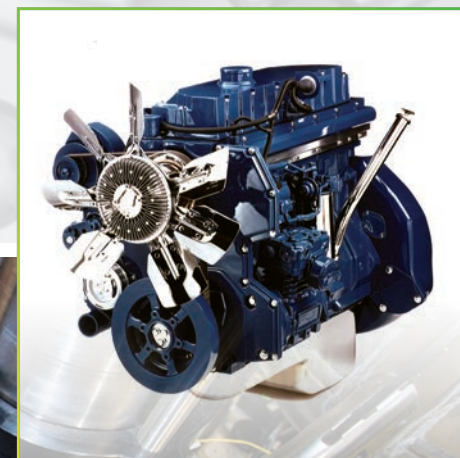
Technical Research Accomplishments & Impact

The petroleum and automotive industries long ago cracked the code on how to design engines and formulate fuels that would meet drivers' performance expectations. But what does it take to maximize the performance, energy efficiency, and environmental attributes of the next generation of advanced fuels and engines? Co-Optima research is pioneering the comprehensive and coordinated science and engineering needed to deliver on all three fronts.

In the first year of this initiative, the integrated multi-lab team has joined forces across disciplines to simultaneously tackle advanced engine development, fuel property identification, renewable fuels production, simulation tool development, life-cycle and techno-economic analyses, and deployment barriers. The Co-Optima team operates according to a central fuel hypothesis: If target values for critical fuel properties that maximize efficiency and reduce harmful emissions for a given engine architecture are identified, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance. This fuel property-based approach is making it possible for researchers to deliver rigorous technical understanding without favoring a specific technology or approach.

The operating requirements for light-duty, medium-duty, and heavy-duty vehicles can differ widely. Co-Optima's two parallel research thrusts make it possible to address this full spectrum of requirements, while also examining short-term and long-term solutions based on SI and ACI strategies.

Highlights on the following pages represent just a selection of the top FY16 Co-Optima accomplishments.



Building the Foundation

Just as the Co-Optima initiative bridges fuel and engine innovation, a body of foundational research spans the two parallel thrust areas, providing the scientific underpinnings for R&D on multiple fronts.

Perhaps the most important of these foundational elements has been the establishment of a central fuel hypothesis that performance in engines is linked to fuel properties. This governing hypothesis has guided researchers in developing screening criteria, surveying hundreds of bio-derived molecules, and creating a fuel property database containing the chemical and physical properties of more than 400 petroleum- and bio-derived blendstocks. Researchers have also defined a robust engine merit function that defines the relationship between key fuel properties and engine efficiency and is being used to assess the validity of the central fuel hypothesis through carefully designed simulations and engine and reactor experiments.

Other activities crucial to the initiative's success have included identification of critical life-cycle, market, and techno-economic metrics and the analyses of the performance of leading bio-blendstock candidates. In addition, researchers have developed modeling and simulation tools that are being used for scenario-based decision analysis and will be essential to defining the fuel/engine options that maximize performance while meeting key sustainability, affordability, scalability, and compatibility metrics.

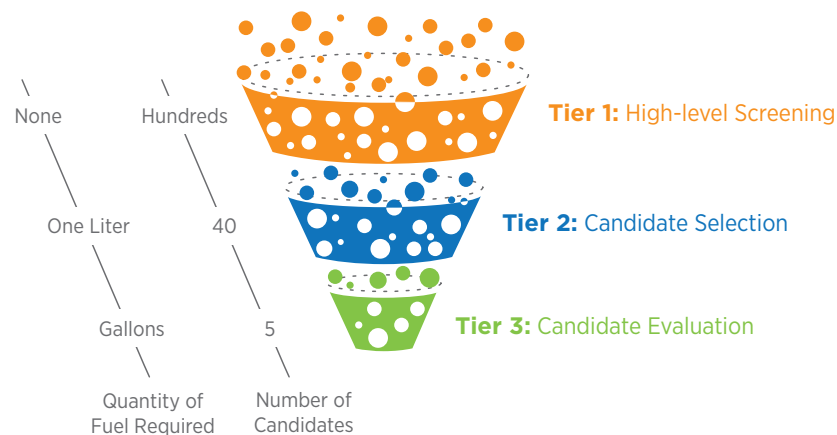
The following section highlights research that provides a foundation for Co-Optima Thrust I and Thrust II activities.

Engine and Fuels Central Hypothesis

If target values for critical fuel properties that maximize efficiency and reduce harmful emissions for a given engine architecture are identified, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance.

Tiered Screening Approach Narrows the Field of Potential Fuel Candidates

Blendstock candidate identification began with a survey of all possible hydrocarbons and oxygenates that can be produced from biomass. Researchers then developed and implemented a tiered screening approach to rapidly identify candidates that have fuel properties advantageous to Thrust I engine operation. The first level ensured the candidates had the requisite chemical and physical properties needed to be blended into commercial fuels. This yielded more than 40 candidates. The second tier involves more detailed property measurements and detailed analyses to identify those that have the potential to improve engine efficiency and be commercially available by approximately 2025. The third tier then involves confirmatory testing and more refined analyses to confirm the potential of the blendstock candidates.



The tiered screening approach began with a high-level screening for suitable chemical properties, followed by detailed candidate selection, which has yielded promising candidates for engine tests.

Assessment of Fuel-Enabled Efficiency Gains Embodied in “Merit Function”

To assist in evaluating promising fuel blendstock candidates, a Thrust I fuel efficiency “merit function” has been developed that estimates the potential gains in engine efficiency associated with changes in key fuel properties. Combined with an assessment of the GHG impacts from the production of the blendstocks, the merit function allows a semiquantitative assessment of the overall GHG reduction potential of various fuel blendstock candidates. Although the function reflects the current knowledge of fuel effects on efficiency, ongoing work within the Co-Optima effort is aimed at refining this knowledge, as well as extending the knowledge through high-fidelity simulations.

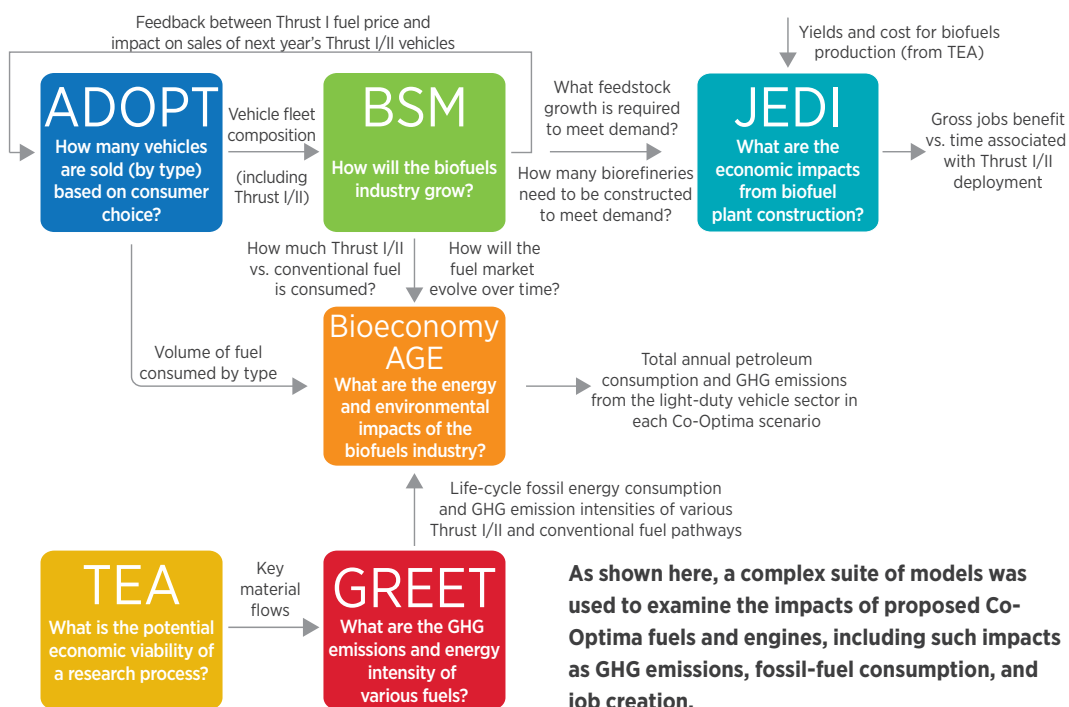
$$\begin{aligned}
 \text{Merit} = & \sum \left[\frac{\text{RON}}{1.6} \left(\frac{\text{RON}_{\text{mix}} - 91}{1.6} \right) + \frac{\text{Octane Sensitivity}}{1.6} \left(\frac{S_{\text{mix}} - 8}{1.6} \right) + \frac{\text{Flame Speed}}{3} \left(\frac{S_{L\text{mix}} - 46[\text{cm/s}]}{3} \right) \right] \\
 & + \frac{\text{Heat of Vaporization}}{1.6} \left(\frac{0.01[\text{ON/kJ/kg}](\text{HoV}_{\text{mix}} - 415[\text{kJ/kg}])}{1.6} + \frac{(\text{HoV}_{\text{mix}} - 415[\text{kJ/kg}])}{130} \right) \\
 & - \frac{\text{Distillation}}{150} \left(\text{LFV}_{150} \right) - \frac{\text{Particulate Emissions}}{0.67 + 0.5(PMI - 2.0)} \left(H(PMI - 2.0)[0.67 + 0.5(PMI - 2.0)] \right)
 \end{aligned}$$

The merit function captures the impact of major fuel properties on the efficiency of an advanced SI engine.

Analysis Assesses the Benefits of Proposed Fuels and Engines

Harnessing a suite of models—including techno-economic, life-cycle, vehicle fleet simulation, biofuel production simulation, and economic impact models—a team of Co-Optima analysts assessed the potential of Thrust I and Thrust II engines and fuels to reduce GHG emissions and fossil-energy consumption in the light-duty sector through 2050. Carried out at the outset of Co-Optima, the analysis estimated a 3%–14% reduction in GHG emissions from the light-duty fleet. The benefits analyses will be expanded and refined during the second year of Co-Optima as more information becomes available regarding the identity and performance of the proposed fuels. Also, the vehicle deployment scenarios will be refined with stakeholder inputs and the scenario expanded to include Thrust II medium- and heavy-duty vehicles.

ASSERT Models: Benefits Analysis



As shown here, a complex suite of models was used to examine the impacts of proposed Co-Optima fuels and engines, including such impacts as GHG emissions, fossil-fuel consumption, and job creation.

Database Is Developed for Bio-Derived Fuel Blendstocks and Their Gasoline Blends

A publicly accessible Fuel Property Database has been created and populated with fuel and chemical property information for candidate bio-based fuel blendstocks. The database focuses on fuel blendstocks (both pure components and mixtures) proposed by the Co-Optima team and is populated with data from literature or measured, and/or predicted data. It currently contains data on nearly 400 bio-based fuel blendstocks. In early FY17, the database will be expanded to include data on blends of the most promising Thrust I blendstocks with both a gasoline designed for such blending a reformulated blendstock for oxygenate blending (RBOB) and a four-component surrogate for RBOB that allows for determining the research octane number (RON) and motor octane number (MON)

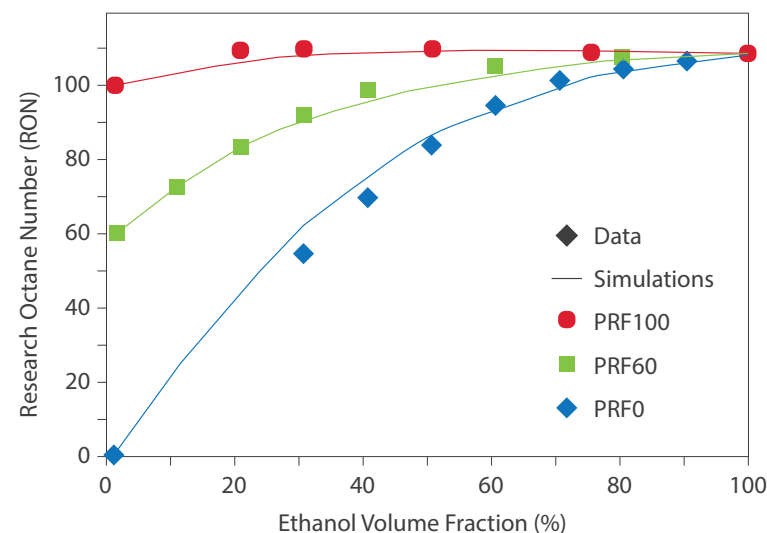
The screenshot shows a web form titled "Found Pure Compound" with a red "Correct or Update this record" button. The form contains the following fields:

- IUPAC name*required: 2-butanol
- Last modified on: 7/6/2016 2:47:30 PM
- Synonyms: sec-Butanol, 2-Butyl alcohol, Methyl ethyl carbinol
- Molecular Weight: 74.12
- Molecular Formula: C4H10O
- CAS#: 78-92-2
- Functional Group: alcohol (dropdown menu)
- Chemical structure: A skeletal structure of 2-butanol with an OH group attached to the second carbon.

The Fuel Property Database includes data on 382 bio-based fuel blendstocks—such as 2-butanol, shown here—and on blends of the most promising Thrust I blendstocks.

Model Predicts Octane Numbers for Blended Fuels with Bio-Derived Components

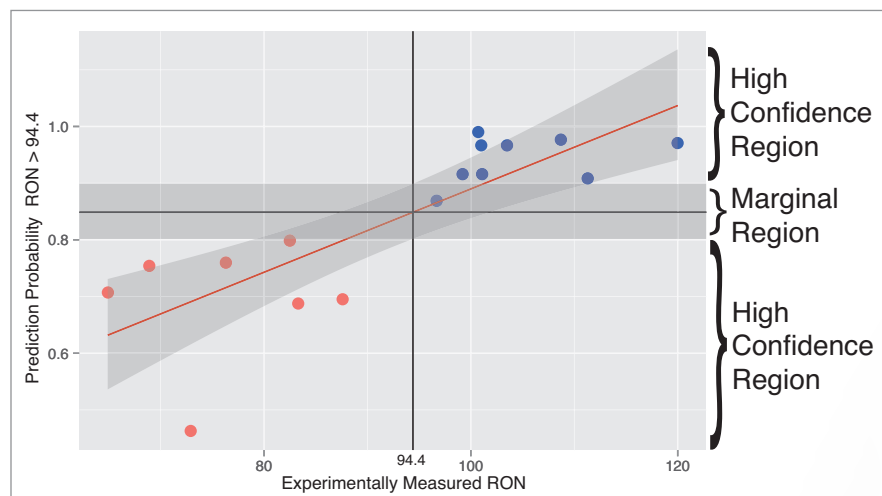
Fuels are generally characterized by important combustion metrics such as RON, MON, and flame speed, but predicting these values for fuel mixtures is difficult because of complex chemical-kinetic interactions that cause non-linear behavior. To address this issue, the Co-Optima team is developing a chemical kinetic model that can predict RON, MON, and flame speed and can model the complex behavior of these mixtures in SI engines. Accurate, validated kinetic mechanisms such as these are critical for developing insight into how fuel properties impact combustion and as inputs to high-fidelity combustion simulations. These results will guide efforts to discover promising bio-derived fuel and gasoline blends that provide the desired ignition and flame speed properties under advanced SI engine conditions.



A newly developed chemical model can predict the RON and MON for blends of gasoline and bio-derived fuels. The predicted RON for ethanol blends is shown here. PRFx are primary reference fuels.

Machine Learning Tool Classifies Fuel Properties in Blendstock Evaluation

Co-Optima researchers developed an open source and general-purpose machine learning tool for classifying fuel properties of biologically produced chemicals. This allows synthetic fuel biologists, chemists, and fuel researchers to rapidly classify, screen, and rank compounds based on their desired fuel properties. Because measuring properties like RON can be intractable for large numbers of chemicals, this tool can dramatically decrease the work in triaging chemicals for experimental validation, potentially leading to new components for fuel blends. In a direct experimental test of this software, using measured RON, the classification predictions provided meaningful leads.



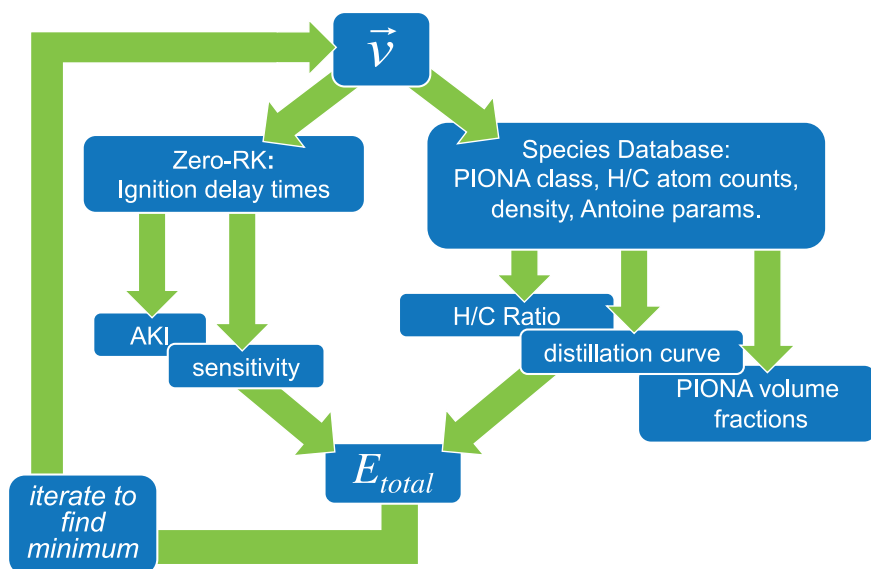
Regression of experimentally measured RON by probability in high RON class (RON > 94.4) for validation compounds. A linear regression of classification probability of RON > 94.4 by experimentally measured RON has an $r^2 = 0.653$ ($P < 0.001$). Based on this relationship, all 16 compounds are correctly classified, with one compound falling away from the 95% confidence intervals of classification (this compound is shown in the horizontal shaded area).

Co-Optimizer Software Solves Merit Function for Fuel Blendstocks

Identifying co-optimized solutions requires assessing the tradeoffs between a number of complex parameters—engine efficiency, environmental performance, infrastructure compatibility, etc. To address this in a systematic manner, a modeling approach has been developed that optimizes fuel component blending to maximize engine efficiency (as defined by the merit function). Users can specify constraints on each of the 21 metrics identified to assess environmental, economic, and infrastructure attributes of the blendstocks in the fuel property database. This type of optimization problem constitutes a difficult-to-solve, mixed-integer, non-linear programming problem. The team has turned to genetic algorithms to generate solutions efficiently and is exploring surrogate optimization to allow complicated blending models that still achieve interactive levels of performance. The team is examining the tradeoff between engine merit function and cost and exploring the impact of a number of factors to understand how potential biofuel blendstocks impact engine performance.

New Tool Automatically Generates Physically Accurate Surrogate Fuel Mixtures

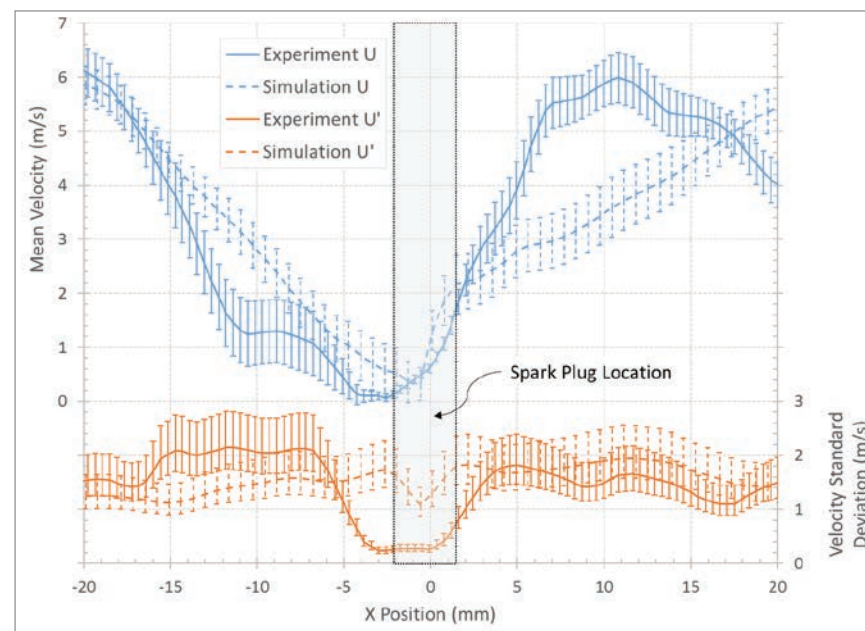
Co-Optima engineers have developed a tool that quickly generates surrogate fuel mixtures to match key physical and kinetic properties of current and proposed fuels, a necessary input into fuel and engine simulations. The “surrogate generator” automates a painstaking process that could only match a few physical properties for one fuel. It employs a fast chemical-kinetic solution method to calculate the fuel’s ignition characteristics, combining that with molecular composition and distillation data to produce better matches to more data in minutes. Using the tool on a supercomputer, it can run in parallel to investigate a wide array of model fuel surrogates.



This flow chart demonstrates how the surrogate generator tool iteratively solves for the surrogate fuel mixture (vector \vec{v} of component volume fractions) that has the “best” match to the experimentally measured properties for the real fuel.

Parallel-Cycle Simulations Yield Fuel Velocity Statistics in Bulk

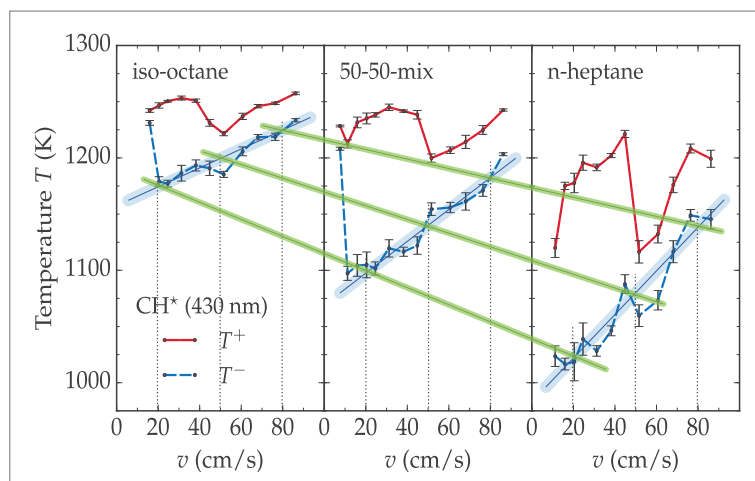
The Co-Optima project has simulated 35 motor engine cycles using a parallel-cycle approach for a pent-roof optical engine. This is the first time this kind of approach has been applied to an engine with non-simplified combustion chamber geometry. With this method, each engine cycle is simulated in parallel rather than sequentially, potentially saving an order of magnitude or more time to complete the simulations. The results show reasonable agreement between particle image velocimetry measurements and simulation results and provide a solid foundation to build upon for simulations of combustion engine cycles.



Comparison of fuel velocity mean and standard deviation data along the x-axis through the spark gap.

Microliter Fuel Ignition Tester Detects Octane Number Dependence

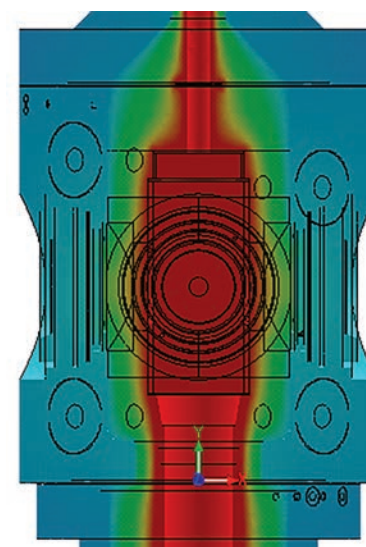
Co-Optima and Louisiana State University have developed a prototype microliter Fuel Ignition Tester (μ FIT), in which premixed fuel and air flow down a small-diameter quartz tube that is externally heated, creating a positive temperature gradient down the length of the tube. This geometry allows a number of steady and unsteady flame dynamics to be established and studied with μ FIT, varying the flow velocity, fuel reactivity, fuel-air ratio, and temperature gradient. With a fueling rate of roughly a microliter per minute, μ FIT can potentially perform rapid fuel screening with sub-microliter samples, providing estimates to the fuel property inputs needed for the engine merit functions. In addition, detailed thermal modeling eliminated a major source of temperature error in the μ FIT system, which is enabling a redesign of the equipment and procedures to make the measurements suitable for more quantitative comparisons.



Flame ignition (red) and extinction (blue) positions at different flow speeds in the μ FIT prototype. The flames become unstable at low flow velocities, entering a mode of repetitive extinction and ignition. In a single cycle, these dynamics provide insight into high-temperature chemical kinetics at the ignition point, low-temperature kinetics at the extinction point, and laminar flame speed. The octane number of the two components and their mixture was found to have a nearly linear correlation to the wall temperature at the point of flame extinction across both stable and unstable flame regimes.

Spray Chamber Simulates Engine Temperatures and Pressures

Co-Optima engineers have designed a spray chamber that will recreate the typical conditions for either gasoline or diesel injection while offering optical access for research needs. The design involved extensive finite element and thermal analysis to achieve an optimal design for the chamber's optical, thermal, and strength performance. When fabricated and installed, the chamber will offer a continuous flow of charge gas at temperature and pressure, allowing fuel effects on spray development to be investigated with up to a 300-fold increase in productivity.



The predicted gas temperature distribution in the spray chamber while pressurized shows that the high-temperature gases at 1,100 K (red) are isolated from chamber walls, which remain at 400 K (blue) to maintain the integrity of the pressure vessel.

Thrust I: Spark Ignition

Spark ignition (SI) engines found in most of today's light duty vehicles use less fuel and produce fewer polluting emissions than cars did 20 years ago, but further advances to these engines and the fuels that power them are needed to maximize efficiency and vehicle performance while reducing harmful emissions. Co-Optima Thrust I activities have focused on identifying fuel properties that can enable market introduction of downsized, turbo-charged SI engines in the 2025 timeframe. More specifically, researchers are mapping the relationships between production pathways, molecular structure, fuel chemical/physical properties, and engine performance.

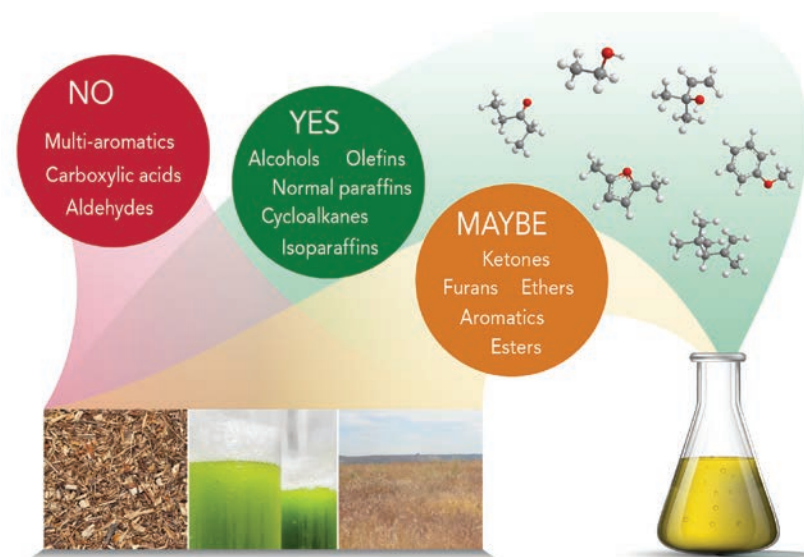
Researchers identified more than 400 blendstock candidates that can be produced via biological or fossil pathways and applied a tiered screening approach to eliminate candidates that had properties unsuitable for use in commercial fuels. This evaluation resulted in identification of more than 40 molecules/mixtures with properties suitable for Thrust I fuel blendstocks. Researchers continue to refine this list to pinpoint those with properties with the greatest potential to enhance SI engine performance.

These assessments are being guided by analyses of 20 representative molecules/mixtures across 21 metrics related to sustainability, economics, scalability, and market viability. Experiments and modeling have provided crucial insights that have improved the understanding of fuel property impacts on SI engine performance.

The following section highlights select Co-Optima Thrust I accomplishments.

Assessment Identifies More Than 40 Bio-Derived Materials as Potential Blendstocks

Co-Optima researchers performed the first systematic assessment of the suitability of oxygenate functional groups in fuel blends for SI engines. The team used a multistep approach that assessed a broad range of chemical functionalities, eliminating those with poor fuel characteristics. This approach allowed the team to identify more than 400 potential blendstocks within the remaining functional groups that can be derived from biomass, including individual molecules and mixtures. The team then applied a tiered screening approach to determine which have a high likelihood of meeting fuel property metrics. Ultimately, the team identified 39 blendstocks with a RON greater than 98 that met Tier 1 screening metrics. The blendstocks were then subjected to further performance and property testing.



The team evaluated the full range of potential bio-derived chemistries, evaluated functional groups that could potentially be fuels, and then identified nearly 400 candidates for further testing. Ultimately, more than 40 compounds and mixtures met the Tier 1 screening requirements and were targeted for additional research.

Analysis Evaluates 20 Thrust I Candidate Blendstocks

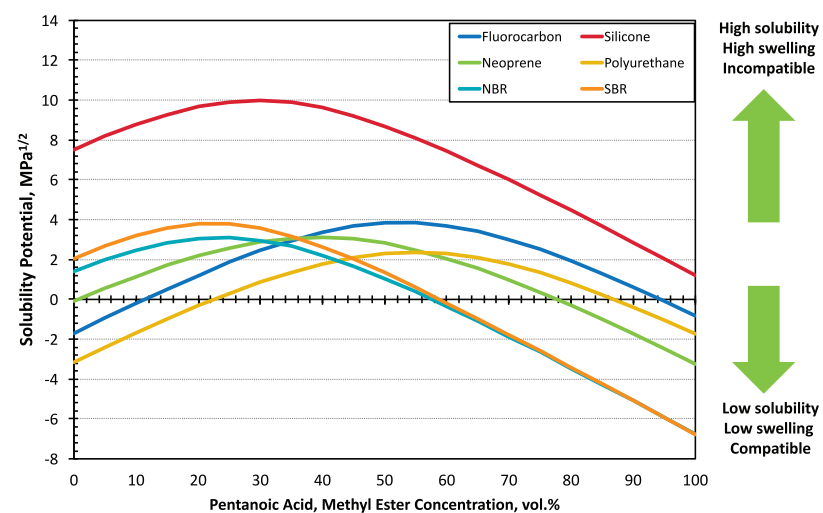
Co-Optima analysts developed 21 metrics in the categories of process economics, technology readiness, sustainability, and market barriers against which to evaluate a subset of 20 promising Thrust I candidate blendstocks with a RON exceeding 98. These metrics include the target cost and state of technology for blendstock production, as well as life-cycle GHG emissions. Such metrics are key to further assessing the viability of candidate blendstocks that meet the required physical properties. Blendstock candidates were assessed at the close of Co-Optima's first year. Five candidates were identified for more rigorous analyses in the project's second year.

Metric	Favorable	Neutral	Unfavorable
Example 1: Target cost (\$/gge)	Falls in lowest-cost grouping of blendstocks	Falls in middle-cost grouping of blendstocks	Falls in highest-cost grouping of blendstocks
Example 2: Life-cycle GHG emissions	Likely to achieve a greater than 60% reduction in life-cycle GHG emissions as compared to conventional gasoline in 2015.	Could achieve a greater than 60% reduction in life-cycle GHG emissions as compared to conventional gasoline in 2015.	Unlikely to achieve a greater than 60% reduction in life-cycle GHG emissions as compared to conventional gasoline in 2015.

Two examples of the 21 metrics for blendstocks—target cost and life-cycle GHG emissions—and the criteria used to rank them as “favorable,” “neutral,” and “unfavorable.”

Compatibility Issues Examined in Analysis of 32 Blendstocks, Six Elastomers

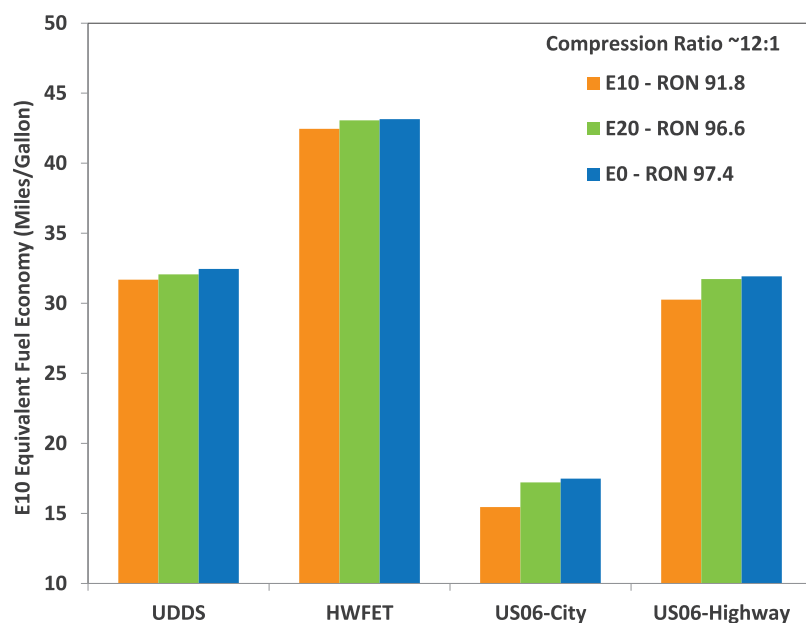
Co-Optima researchers have examined the compatibility of 32 fuel candidate blendstocks with six elastomers, using a theoretical chemical method called the Hansen solubility analysis. The blendstocks were evaluated for blends with dodecane (representing gasoline) and E10D (representing 10% ethanol blends), and the results show that the blend level has a significant impact on compatibility. For many candidates, the solubility potential (or potential swelling) increases with higher blendstock content and peaks at low- to mid-range concentrations. For many elastomers, the solubility is within an acceptable range, but experimental testing will be undertaken in FY17 to confirm their compatibility.



Solubility analysis results for pentanoic acid and methyl ester demonstrate that blend levels can have a significant impact on solubility, although for many elastomers, the solubility is within an acceptable range.

High-Octane Blends Improve Fuel Efficiency in Aggressively Tuned Engines

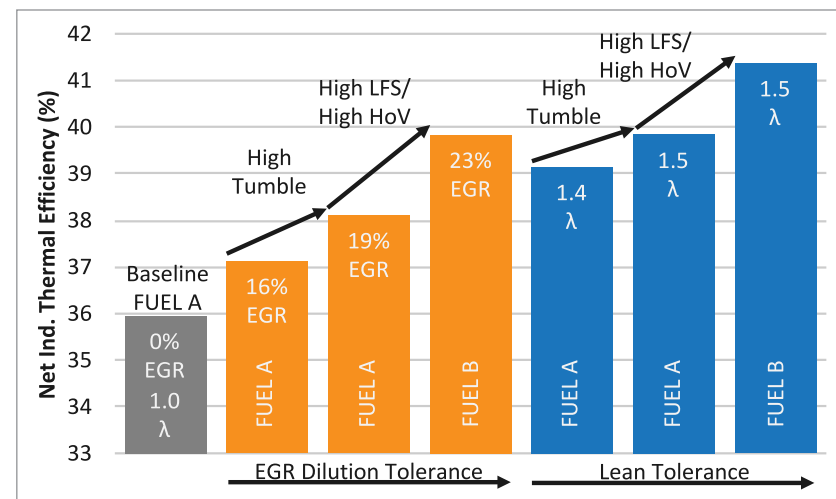
At a compression ratio of 12:1, use of 98 RON fuels (including E20) yields significant fuel efficiency improvements relative to 92 RON fuel, offering the possibility of fuel economy parity with E10 fuels for some driving cycles. The benefit of octane increases with the aggressiveness of the driving cycle due to the higher fraction of time spent in knock-limited combustion phasing conditions. Higher RONs reduce the need to retard combustion phasing under these conditions, improving fuel efficiency. Engine downsizing and down-speeding are well suited to take advantage of higher-octane fuels because these engines encounter the knock limit more frequently.



E10-equivalent fuel economy results for the three study fuels at a compression ratio of 12:1 show fuel economy benefits for fuels with higher RONs.

Higher Fuel Laminar Flame Speed Expands Dilute or Lean Operation

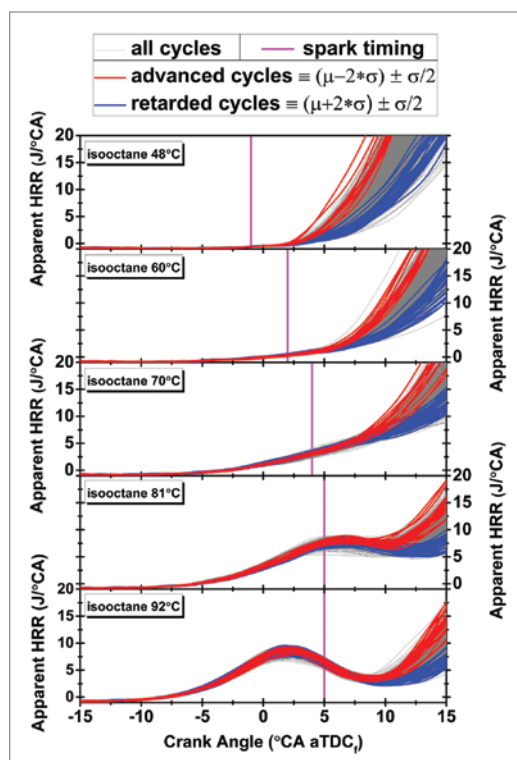
Five fuel blends (all based on pure components) were designed to test the effect of laminar flame speed (LFS) on the lean and exhaust-gas recirculation (EGR) dilution limits of SI combustion with various constant heats of vaporization (HoV). While having a low HoV is important for stable combustion, the higher LFS is also important because it allows for leaner mixtures or increased EGR dilution even while the HoV is high. Compared to typical engine design parameters (spark energy, tumble ratio, and direct injection (DI)), fuel LFS had similar impacts on lean and EGR-dilute SI combustion limits.



Increased fuel LFS allowed higher EGR dilution and lean tolerance, resulting in improved engine indicated thermal efficiency. Fuel LFS effects were as significant as changes to key engine design parameters.

Boost Can Cause Pre-Spark Heat Release in SI Engines

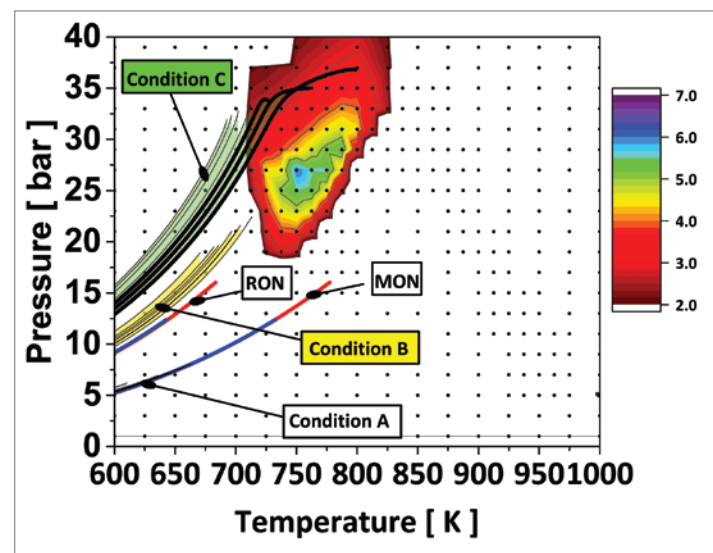
Operation under boosted conditions is essential to Co-Optima's Thrust I effort to maintain acceptable power density for downsized and downsped SI engines. However, boosted engines encounter temperature and pressure conditions that are not seen in naturally aspirated engines, which constitute the majority of today's SI engines. These boost conditions are also well outside the range experienced in either the RON or MON tests. Investigations revealed that with sufficient boost, some fuels exhibit heat release prior to SI. This behavior may have far-reaching implications on understanding the boundary conditions for engine knock and other abnormal combustion phenomena.



Pre-spark heat release development as the intake temperature is increased with iso-octane under boosted conditions in a stoichiometric SI engine.

Kinetic Simulation Provides Insight to Pre-Spark Heat Release

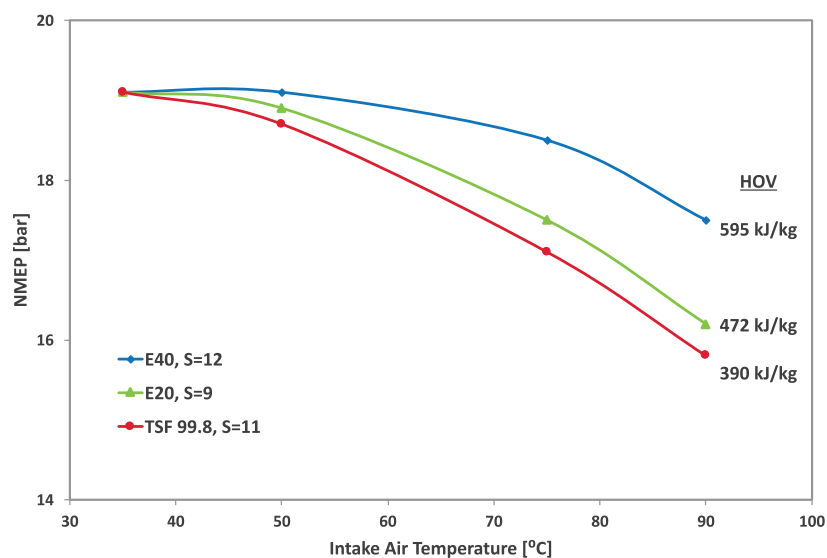
Co-Optima is successfully applying chemical-kinetic modeling to provide insight into the regions of reactivity and how that relates to different fuels. Experimental temperature and pressure traces combined with kinetic simulations of autoignition chemistry are demonstrating how boosted operating conditions interact with regions of enhanced reactivity at highly boosted conditions. Specifically, pre-spark heat release is observed in stoichiometric SI engines with some fuels at conditions that are important for Thrust I technologies. This method can provide insight into Co-Optima paths for fuel compositions and operating conditions as the project moves forward.



An island of low temperature heat release (LTHR) was identified in the pressure/temperature space using kinetic simulations and is presented using the contour plots above. The lines depict the compressive process in the temperature/pressure space for different operating conditions. The investigation found that the highest load condition (Condition C, green) is the only operating condition that interacts with the LTHR island and, as a result, is the only operating condition to exhibit pre-spark heat release.

Fuel HoV Influences the Knock Limit at High Intake Temperatures

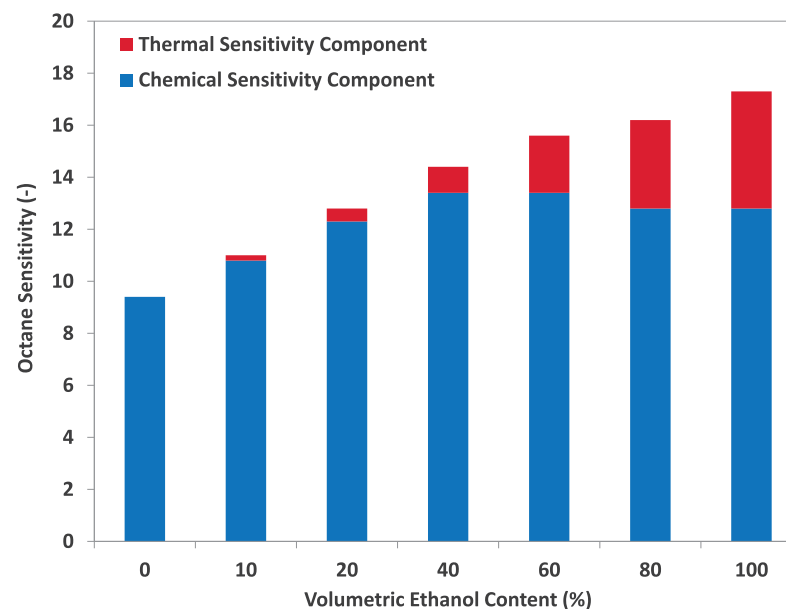
The RON and octane sensitivity of a fuel are closely associated with its knock resistance, but recent research has found that the fuel's HoV plays a role at high intake air temperatures. Research with a single-cylinder, gasoline DISI engine at a fixed retarded combustion phasing and intake air temperatures higher than 60°C found that fuels with higher HoV values enabled operation at significantly higher load. This important Co-Optima research decouples the physical HoV effect from the RON and octane sensitivity effects, and for the first time, demonstrates engine operating conditions where HoV effects on knock resistance can be measured.



Knock-limited loads at late combustion phasing (CA50 = 20.5° ATDC) are shown with 100 RON fuels. At higher intake air temperatures, fuels with higher HoVs allow higher loads to be achieved.

HoV Contributes to Octane Sensitivity

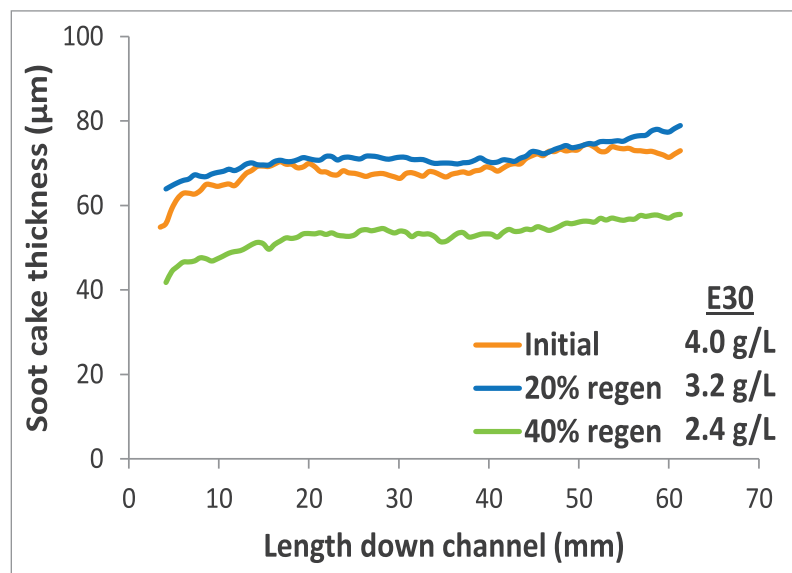
Increasing the latent HoV of gasoline blendstocks has the potential to increase fuel knock resistance in DI engines. However, studies that fix the octane sensitivity find that HoV does not produce an additional anti-knock benefit. Two new studies were performed to further investigate the relationship between HoV and octane sensitivity. One study found similar combustion phasing under knock-limited spark advance (KLSA) conditions for three similar fuels with differing HoVs, while a second study found that KLSA is well correlated with the RON. The study results indicate that HoV anti-knock effects can be viewed as a contributor to octane sensitivity.



Chemical and thermal components of octane sensitivity derived from Foong's work at the University of Melbourne shows that the HoV contributes to octane sensitivity at high concentrations of ethanol.

Particulate Matter from Ethanol Blends Has Lower Activation Energy than from Gasoline

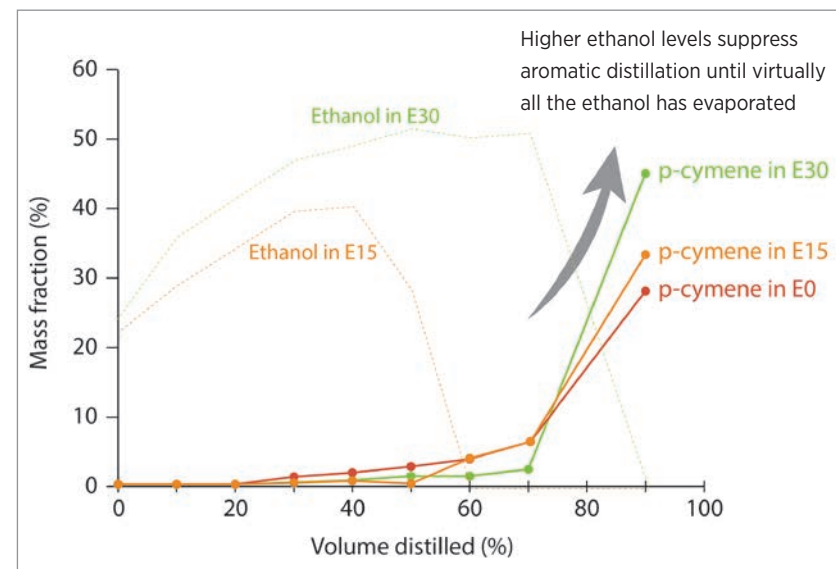
Co-Optima has determined that Thrust I fuel blends will likely influence particulate matter (PM) oxidation behavior in the absence of an aftertreatment solution, which could have regulatory implications. Gasoline particulate filter (GPF) cores were exposed to exhaust from a DI engine running on either 100% gasoline (E0) or a 30% blend of ethanol in gasoline (E30). Subsequent measurements were done with neutron imaging. As shown below, it was determined that the thickness of the PM soot cake did not change until 20% of the carbon had been removed with little difference between fuels. While the E30 PM was easier to oxidize, both the E0 and E30 PM oxidize differently than diesel PM.



Studies with GPF cores show the presence of organic fraction, increasing the activation energy for oxidation.

Possible Link Found Between Particulate Matter and Ethanol's Interaction with Aromatics

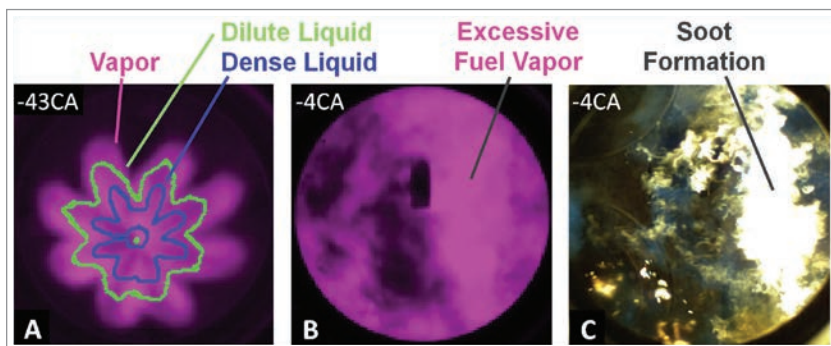
Co-Optima researchers characterizing a set of 15 gasoline blends made the unanticipated discovery that ethanol suppresses aromatic evaporation and pushes it to higher temperatures. Incomplete fuel vaporization and mixing produces higher PM emissions—especially for aromatic compounds with a high sooting tendency. E15 or E30 blends inhibited evaporation of the aromatic at the midpoint of the distillation curve, causing the fuel to be enriched with the aromatic toward the end of the distillation. In ongoing work, the Co-Optima project is testing these fuels in a DISI engine to measure PM emissions.



Distillate composition results for 10% by volume blends of p-cymene in E0, E15, and E30 demonstrate a suppressed aromatic distillation until a large fraction of the ethanol has evaporated.

Imaging Reveals Mechanism for Smoke Emissions at Higher Engine Speeds

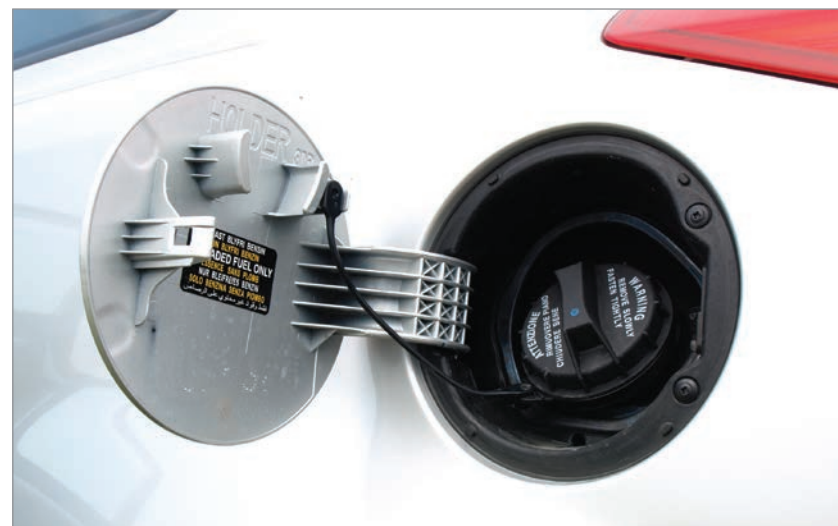
Spray-guided stratified-charge operation of SI engines is one approach to lean operation, which yields higher efficiency. However, fuel stratification may lead to excessive smoke emissions. Co-Optima researchers employed several optical diagnostics in a DISI engine that used in-cylinder swirl to stabilize the combustion at higher speeds. A new high-speed infrared fuel-vapor imaging technique demonstrated that tumble flows are generated in conjunction with the swirl and create asymmetric fuel distributions, leading to excessively rich gas volumes that promote soot formation. This research may lead to clean and efficient stratified-charge SI engine operation and guide the formulation of new high-octane gasoline fuels.



Infrared fuel-vapor images during gasoline fuel injection (a) and at the time of the main combustion phase (b). Green and blue contours correspond to dilute and dense liquid boundaries detected by a separate Mie-scattering technique. The last image (c) shows an example of soot luminosity caused by tumble-induced fuel-vapor asymmetry.

Committee Tackles Standards for Electronic Misfueling Mitigation Technologies

When vehicles designed for new fuels are accidentally fueled with incompatible legacy fuels, or vice versa, it can result in serious vehicle performance issues and potentially irreparable damage. Misfueling mitigation strategies can prevent these mistakes. Of all available techniques, electronic misfueling mitigation technologies that would enable wireless communication between the vehicle and the dispenser appear most effective. Yet such an approach would require the development of new technical standards. Input from automotive and fuel retailing stakeholders has underscored the need for such a standard and an investigation of related factors. The Co-Optima program plans to assemble a committee to accelerate the establishment of needed mitigation strategies.



Fuel-grade guidance labels, whether inside the filler door or on the pump, are less effective than mechanical or electronic means of preventing misfueling. For Co-Optima fuels, more foolproof strategies are needed.

Thrust II: Advanced Compression Ignition

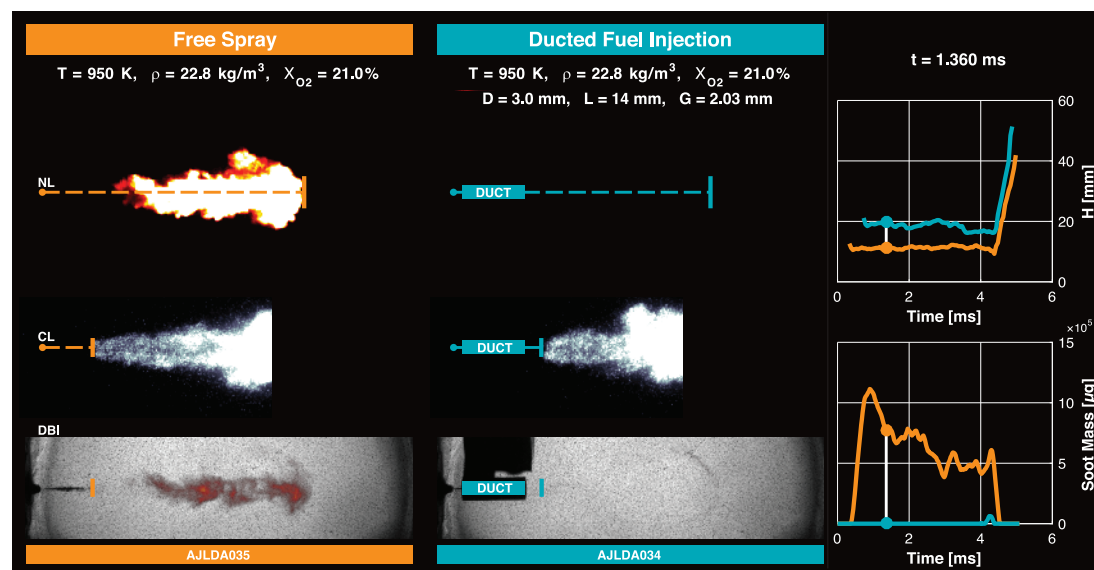
Even if the performance of SI engines is taken to the limit, greater efficiency improvements can be realized through commercialization of ACI technologies. Co-Optima Thrust II research efforts are exploring the factors important for enabling ACI technologies, along with the supporting fuel technologies necessary to produce a higher-impact series of solutions.

Engine and fuels performance researchers have been working hand-in-hand to identify fuel properties that critically impact kinetically controlled combustion and LTC. In addition, they are mapping the interplay of molecular structure, fuel properties, engine design, and operating strategies needed to enable high-efficiency ACI engine operation across a broad range of applications. Researchers are using Thrust II engine simulations with detailed combustion kinetics to assess fuel property effects in conditions beyond the range possible with Thrust I engine experiments.

The following highlights provide more detail on these Thrust II accomplishments.

Ducted Fuel Injection Reduces Soot from Mixing-Controlled Combustion

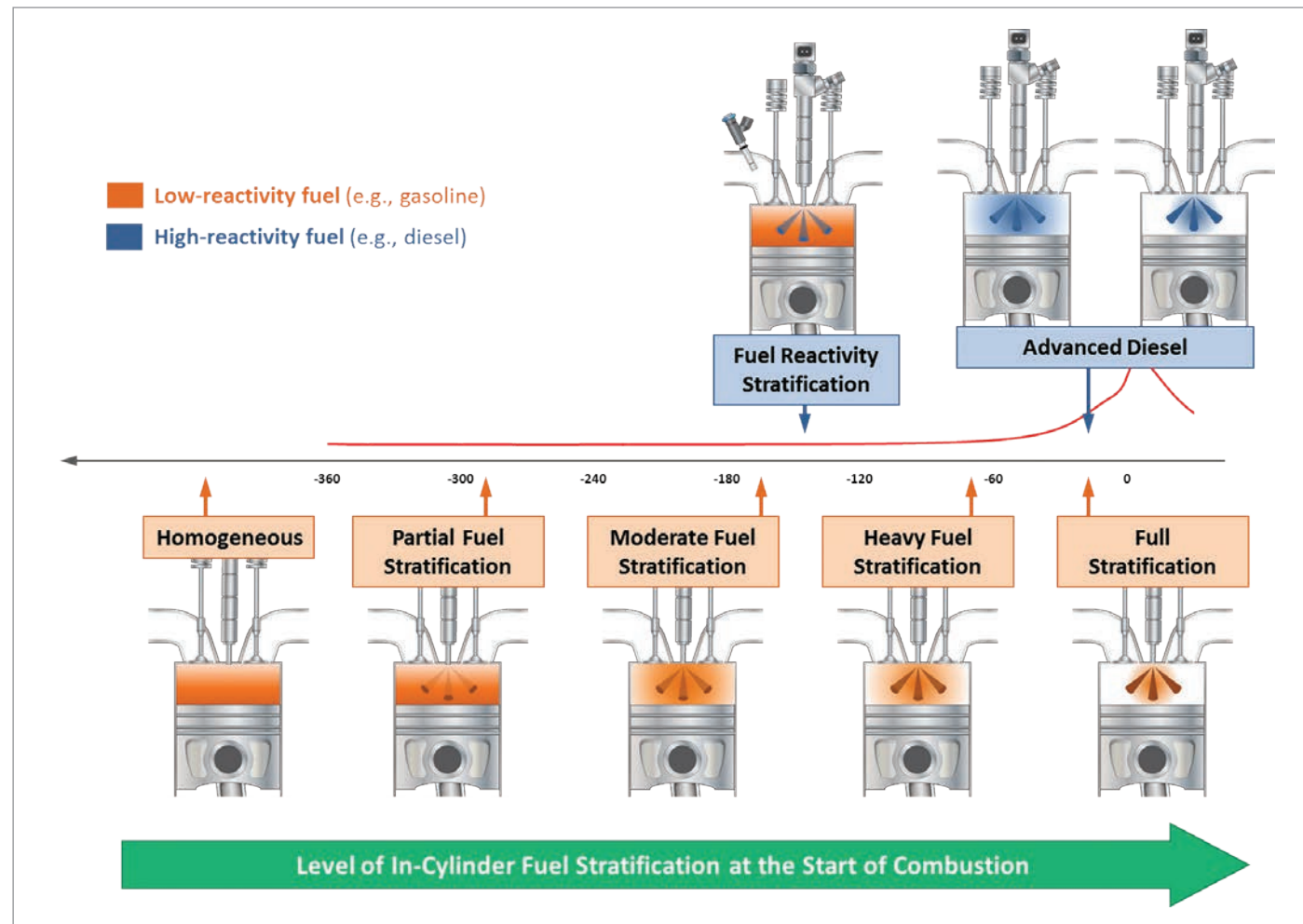
The Co-Optima project employed constant-volume combustion-vessel experiments to measure soot reductions enabled by a variety of ducted fuel injection (DFI) configurations studied over a range of ambient temperatures (850 K–1,200 K), densities (14.8 and 22.8 kg/m³), and oxygen mole fractions (15% and 21%). Soot was typically reduced by half to more than two orders of magnitude, depending on ambient conditions and duct configuration. DFI could be a key Co-Optima technology because it is an effective, simple, mechanical approach that is not highly sensitive to the use of dilution for control of nitrogen oxides (NO_x) or to fuels having significant variability in their properties. This discovery has particularly important implications to compression ignition engine technologies, which are efficient but have sooting challenges.



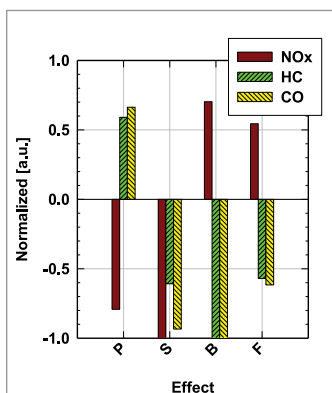
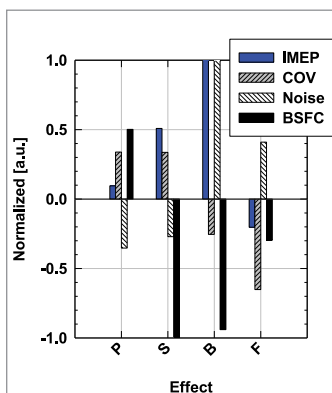
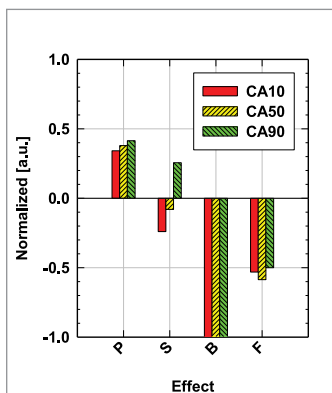
Under mixing-controlled combustion of a free spray vs. DFI, the natural luminosity (NL) image in the top row shows an absence of hot soot with DFI, which is supported by the absence of any soot in the corresponding diffuse back illumination (DBI) image in the bottom row. The OH* chemiluminescence (CL) images in the middle row show that there is indeed robust combustion with DFI, and the time-resolved lift-off length, H , is determined from these images (upper right plot). The plot in the lower right corner shows that the total soot mass as determined by DBI is 5 to >100 times lower with DFI relative to the free spray.

In-Cylinder Fuel Stratification Is Key to Classifying Advanced Combustion Modes

Co-Optima researchers have developed a new perspective on ACI combustion strategies by classifying them along a spectrum that features increasing degrees of air and fuel stratification at the start of combustion. This new perspective unites how all of these previously thought “individual” combustion modes relate to one another along this spectrum. This perspective of investigating low-temperature combustion on a continuum of in-cylinder stratification is critical to informing new research efforts focused on achieving potential efficiency gains and emissions reductions with these related modes, perhaps offering researchers more flexibility in expanding ACI to cover wider engine operating load ranges.



ACI combustion strategies are shown as a continuum based on the level of fuel stratification at ignition, with gasoline compression-ignition modes on the bottom and advanced diesel and dual-fuel ACI modes on the top.



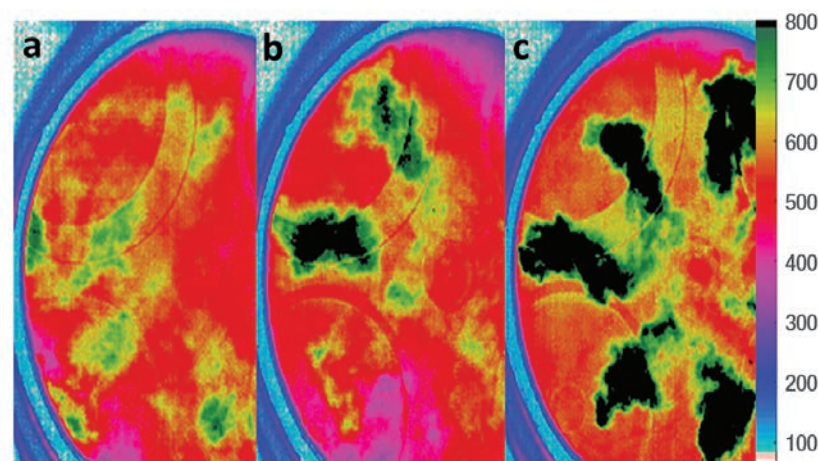
Study Finds Engine Designs that Promote Stratification Can Yield Reliable Autoignition

Co-Optima engineers tested two fuels with different anti-knock properties—one similar to E10 and the other similar to a naphtha distillate—finding that the boost level had the most significant impact on autoignition, while stratification was just as important as the fuel choice. The results will help develop clean, efficient engines that can burn fuels with variations at the pump. Knowledge of such fuel properties will allow future engines to employ injection parameters, EGR, and boost to create reliable autoignition.

Fuel property results at 2,000 rpm/ $\lambda=3$, testing the influence of injection pressure (P), start of injection (S), boost (B), and fuel (F) upon three main groups of effects: Crank angles of 10%, 50%, and 90% (CA10, CA50, and CA90, respectively); indicated mean effective pressure (IMEP), the coefficient of variation (COV) in IMEP, noise, and brake-specific fuel consumption (BSFC); and emissions of nitrous oxides (NO_x), hydrocarbons (HC), and carbon monoxide (CO). The y-axis shows the relative significance of each factor compared to the other factors. Longer bars signify more influence of that parameter upon the measurement listed, while shorter bars mean the factor has little or no influence upon the measured parameter.

Infrared Combustion Imaging Aims to Extend RCCI Load Limits

The Co-Optima project is employing infrared imaging to improve the understanding of in-cylinder mixing and fuel-property effects on ignition and combustion processes in reactivity-controlled compression ignition (RCCI) combustion. RCCI experiments are being coordinated between two laboratories with overlapping sets of operating conditions that vary premixed-fuel fraction and DI timing. The infrared images show how different in-cylinder fuel distributions correlate to different pressure-rise rates, which currently limit high-load operation of RCCI engines. These imaging results provide guidance for targeting specific operating conditions for more detailed and quantitative laser-based fuel-tracer fluorescence diagnostics to measure fuel concentration and temperature in FY17.



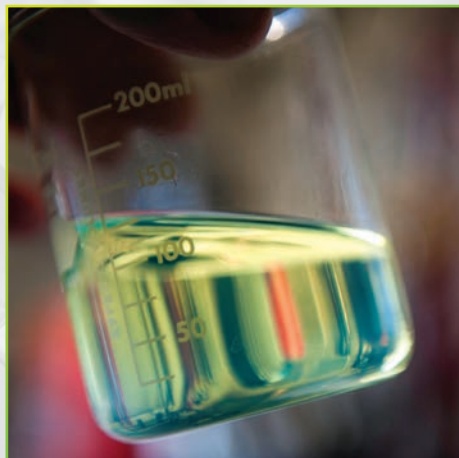
Infrared images of thermal emissions from hot in-cylinder fuel and combustion products for three different modes of RCCI combustion: (a) early injection timing, with distributed ignition and modest pressure rise-rates; (b) intermediate injection timing, with localized (mixture preparation controlled) ignition and high pressure-rise rates; and (c) late injection timing, with jet-mixing-controlled combustion similar to conventional diesel combustion and modest pressure-rise rates.

Next Steps

The Co-Optima team is looking forward to significant developments in the year ahead. The team plans to assess the validity of the central fuel hypothesis by the project's 18-month mark. It is anticipated that at least three bio-based candidates will have passed screening as potential Thrust I blend components and demonstrated engine performance comparable to that of a petroleum-derived fuel.

At that time, Thrust I blendstock discovery efforts will be considered complete, and a decision will be made to determine the relative research priorities needed to accelerate delivery of Thrust I fuels and advanced engines to the market. This decision point will involve an end-to-end scenario-based analysis defined through engagement and discussions with stakeholders.

Work on Thrust II ACI R&D will press forward, with experiments, simulations, and analyses planned to identify how fuel properties and ACI operating strategies can be co-optimized to achieve the high efficiency and low-emissions potential of these combustion approaches. Thrust II R&D will be enhanced through new collaborations with the nation's top universities. Eight university teams will work with Co-Optima researchers to carry out fundamental studies to complement the work being done at the national labs.



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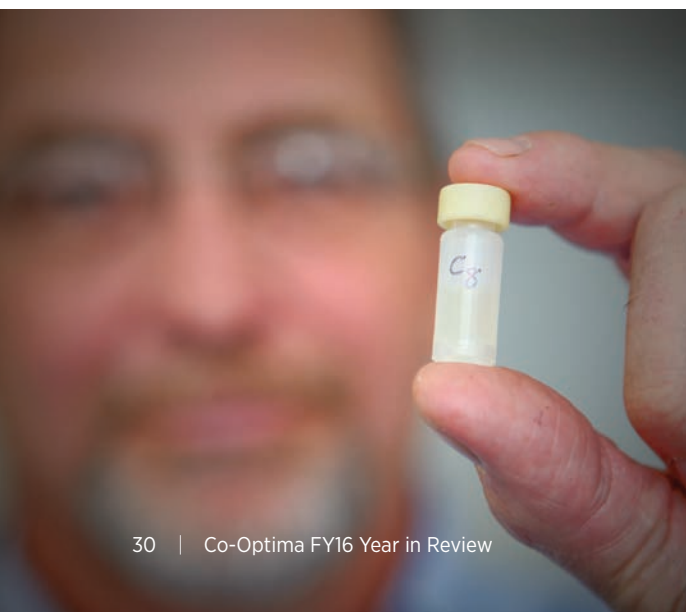
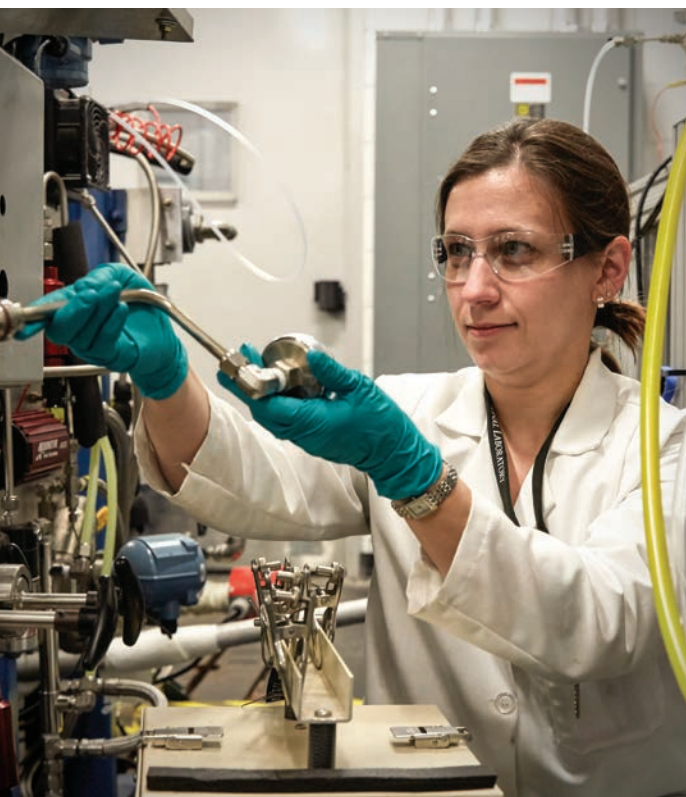
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