ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

CO-OPTIMIZATION OF FUELS & ENGINES

FY17 YEAR IN REVIEW

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

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

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

LETTER FROM THE LAB LEADERSHIP TEAM/EXECUTIVE SUMMARY

Researchers from national laborato
versities across the United States
their combined scientific might be
Co-Optima Initiative, conducting t
ly-stage research needed to accelerate the
of advanced fuel and engines technologies
members are exploring synergies across a
engine, and powertrain options, with a foc
portunities to increase fuel diversification
greater flexibility for refiners and fuel proc

We have adopted a composition-agnostic
identify new blendstocks that can be comb
conventional petroleum-based fuels to del
cantly improved performance in advanced
combustion engines. In fiscal year 2017 (F
research expanded to encompass solution
entire on-road fleet, from light-duty passe
heavy-duty freight trucks.

This report spotlights some of FY17's most
Co-Optima accomplishments. Major highli
past year have included:

- Establishing an improved merit function that quantifies how fuel properties impact boosted spark ignition (SI) engine efficiency
- Identifying representative blendstocks from five chemical families that provide the key fuel properties needed for high-efficiency SI engines
- Screening a wide range of blendstocks to assess compatibility with vehicles and infrastructure
- Determining relationships that describe how chemical structure impacts key fuel properties
- Developing new numerical algorithms and computa- l tools that accelerate R&D
- pleting integrated, systems-level analyses of dstocks in relation to economic, technological, et, and environmental factors.

urse of improving vehicle performance and
y, Co-Optima researchers are also intent on
g a number of broader related benefits. Analysis
o-Optima team indicates that if the goals of the
are realized, then improved fuel economy will
tens of billions of dollars in annual cost savings
ricans. In addition, producing blendstocks from
c biomass resources has the potential to increase
, support rural economies, and keep energy dol-
merica—which ultimately enhances U.S. energy
security and resiliency.

We thank EERE's Vehicle Technolog
and Bioenergy Technologies Office
collaborative support of this initiati
transformative knowledge, data, an
move industry, consumers, and the
sustainable transportation future.

John Farrell
National Renewable
Energy Laboratory

Robert Wagner
Oak Ridge
National Laboratory

John Holladay
Pacific Northwest
National Laboratory

Chris Moen
Sandia National
Laboratories

OPPORTUNITIES FOR NATIONAL IMPACT

Co-Optima R&D is providing U.S. industry with the knowledge needed to maximize vehicle performance and efficiency and leverage domestic fuel resources. This includes the potential to stimulate economic growth and strengthen energy security, while giving American consumers more affordable, fuel-efficient transportation options. All opportunity metrics are based on the Co-Optima team's analysis in relation to 2015 baseline data.

Add up to 500,000 new jobs to spur U.S. economic growth

Cut up to $5 billion in annual fuel costs of heavy-duty vehicles

Boost passenger vehicle fuel economy by 35%

Save $20-$30 billion each year through improved light-duty vehicle fuel efficiency

Maximize use of $1 trillion in existing U.S. fuel infrastructure

Increase supply of domestically sourced fuel by up to 25 billion gallons/year

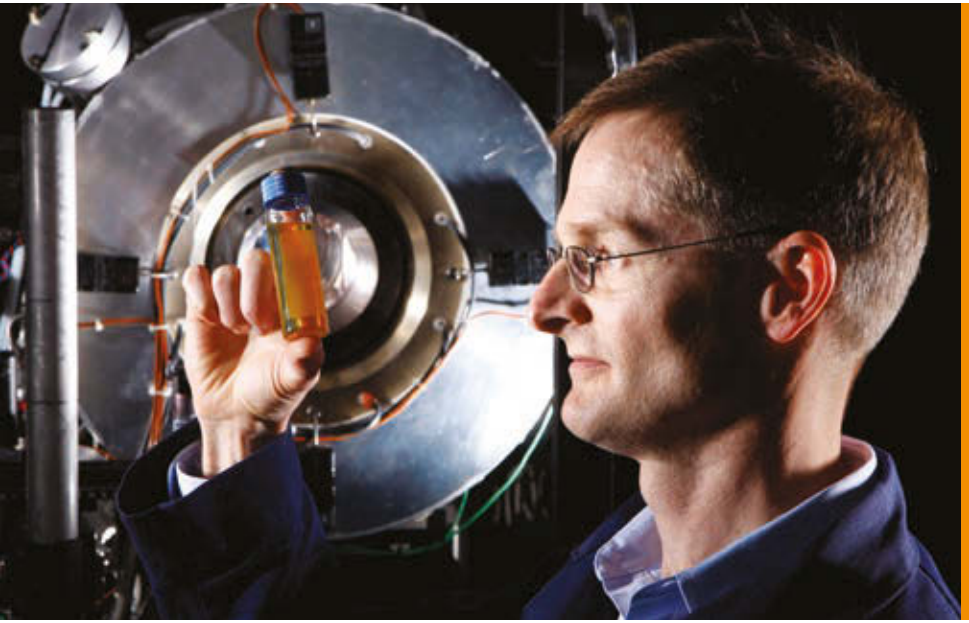
TECHNICAL RESEARCH ACCOMPLISHMENTS & IMPACT

While vehicles and fuels currently on the market get travelers from Point A to Point B, are there new options that could save fuel and money, while also delivering higher performance and cleaner air? Co-Optima research is exploring ways to do just that, with the science and engineering needed to create engines and fuels that work more effectively together.

Co-Optima researchers are considering blendstocks that can be produced from a wide variety of renewable and fossil resources, with a focus on options that can be sourced from domestic cellulosic biomass and similar renewable, non-food, and surplus resources. The blendstock production, fuel property, and engine performance data uncovered through the Co-Optima initiative are making it possible to conduct a detailed assessment of bio-derived blendstocks and identify areas where further R&D is most likely to net meaningful results.

With light-duty vehicles, researchers are investigating ways to improve near-term efficiency through the identification of fuel properties and design parameters that maximize performance for spark ignition and multimode combustion approaches. For medium- and heavy-duty vehicles, the focus is on reducing engine-out emissions while maintaining or improving efficiency in advanced compression ignition approaches.

Highlights on the following pages represent a selection of the top FY17 Co-Optima accomplishments.



CHEMICAL FAMILIES IDENTIFIED FOR CRITICAL FUEL PROPERTIES

Studying compounds from an initial pool of more than 470 candidates, Co-Optima researchers explored how molecular structure affects research octane number (RON), octane sensitivity (S), and heat of vaporization (HOV)—the fuel properties with the greatest impact on engine efficiency for boosted spark ignition (SI) engines.

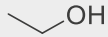
Application of an engine efficiency merit function led to the identification of five chemical families—alcohols, ketones, furans, alkenes, and aromatics mixtures—that impart the desired chemical and physical properties needed to maximize boosted SI engine efficiency. Fuels can be produced using blendstocks from any of these five families mixed with a petroleum base. Ultimately, markets will dictate what blendstocks provide the greatest commercial value proposition.

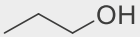
The figures below provide more information on the blendstock candidates, as well as the core and surrogate fuels used in Co-Optima research. Detailed information on the chemical families and the merit function can be found in the Co-Optima studies *Fuel Blendstocks with the Potential to Optimize Future Gasoline Engine Performance and Efficiency Merit Function for Spark Ignition Engines* go.usa.gov/xQx49.

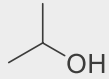
Candidate Blendstock Families

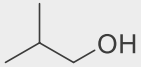
Representative blendstocks from five chemical families identified by Co-Optima researchers as imparting desired fuel properties.

Small Alcohols

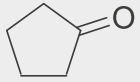

ethanol


n-propanol

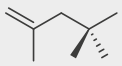

isopropanol


isobutanol

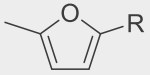
Ketones


cyclopentanone

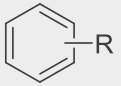
Branched Olefins


di-isobutylene

Furans


R= H, -CH_3
furan mixture

Aromatics



Core Fuels

Five full boiling range fuels with the same RON but different chemical composition used by Co-Optima researchers to allow comparison of results across different labs and experimental platforms.

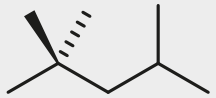
	Alkylate	E30*	Aromatic	Cycloparaffin	Olefins
RON	98	98	98	98	98
Motor Octane Number (MON)	97	88	87	87	88
Anti-Knock Index (RON+MON)/2	97	93	93	92	93
Sensitivity (RON-MON)	1	10	11	11	10
Aromatics (vol%)	1	17	46	32	15
Olefins (vol%)	0	5	4	1	32
Paraffins (vol%)	99	39	41	41	49
Cycloparaffins (vol%)	0	7	8	25	3
Ethanol (vol%)	0	32	0	0	0

**E30=30% ethanol blended in xx.*

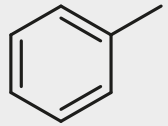
Surrogate Fuels

Simple mixtures of up to 10 molecules used to simulate the chemical reactivity of a full boiling range fuel. The simplified composition allows detailed kinetic simulations to be conducted.

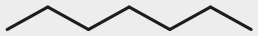
iso-octane



toluene



heptane



1-hexene

This represents just four of the surrogate components being used for blend RON and MON measurement.

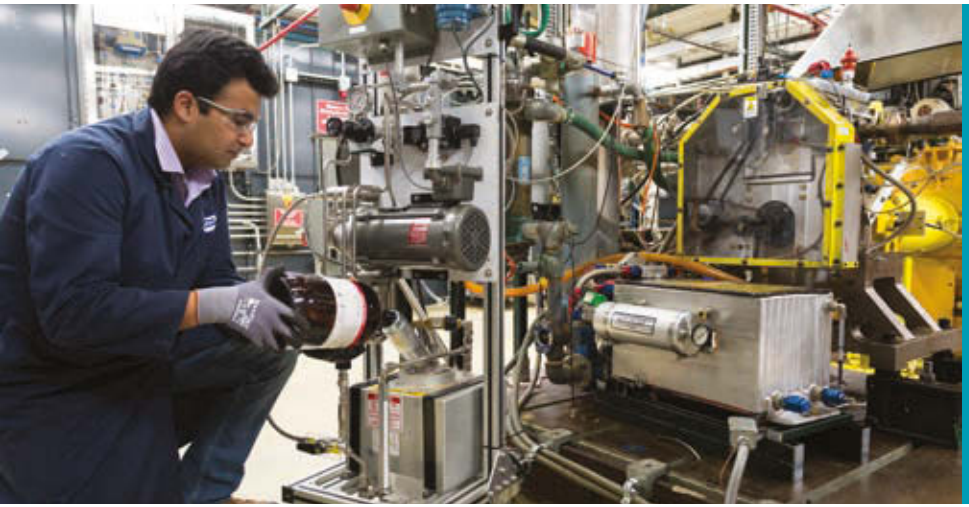
LIGHT-DUTY VEHICLE RESEARCH

While automakers are now offering sophisticated high-efficiency turbocharged engines for light-duty vehicles (LDVs), the maximum efficiency of these engines is currently constrained by fuel properties. Co-Optima researchers are exploring how to maximize performance and minimize emissions through a systematic understanding of the relationships between fuel properties and engine operating parameters.

Researchers are identifying blendstocks that can be combined with conventional petroleum-based fuel to maximized turbocharged ("boosted") spark ignition (SI) engine performance. In addition to having identified representative blendstocks from five chemical families with properties that allow for high efficiency, researchers have applied their analytical expertise to explore production pathways and assess economic, environmental, technological, and market factors. Now, the Co-Optima team is taking this a step further, with researchers assessing fuels for compatibility with polymers, plastics, and metals used in vehicles, as well as the equipment and infrastructure used to produce, transport, and dispense fuels.

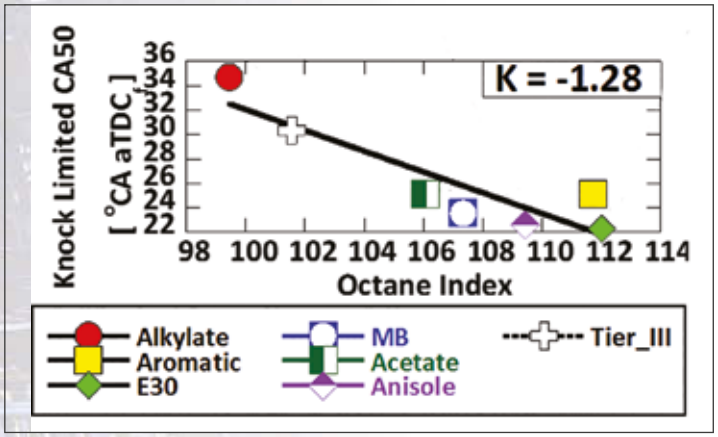
Identifying a co-optimized boosted SI fuel/engine system is an important first step for improving fuel economy, reducing operating costs for the consumer, and improving market viability. However, even greater cycle efficiency and fuel savings are possible with multimode engine strategies that use different methods of ignition, combustion, and/or fuel preparation strategies depending on engine needs. Co-Optima researchers are considering approaches including multi-mode high dilution SI and advanced compression ignition (ACI), along with the fuel properties needed to deliver each option's optimal performance.

Select Co-Optima accomplishments related to LDVs can be found in the following section.



SI Knock-Propensity Experiments Support the Central Fuel Hypothesis

Co-Optima's central fuel hypothesis states that appropriate fuel properties indicate the fuel's performance, regardless of the fuel's chemical composition. To test the hypothesis, Co-Optima researchers studied seven fuels in an SI engine under boosted operating conditions to determine if knock propensity is predicted by fuel anti-knock metrics. The fuels span a wide range of properties and chemistries, including oxygen functionalities not typical for current market fuel. Octane index (OI = RON – K * S), which encompasses the three most important terms in the boosted SI merit function—research octane number (RON), a constant depending on engine design and operating conditions (K), and octane sensitivity (S)—was found to correlate well with knock performance for all fuels, including those with unconventional chemistry. RON and the anti-knock index, however, did not correlate with knock under most conditions. The results suggest that when OI is selected as the property that characterizes autoignition, the central fuel hypothesis is valid. Further studies are underway that identify operating conditions under which the hypothesis breaks down and will shed light on the thermo-physical states where new fuel property understanding is needed.

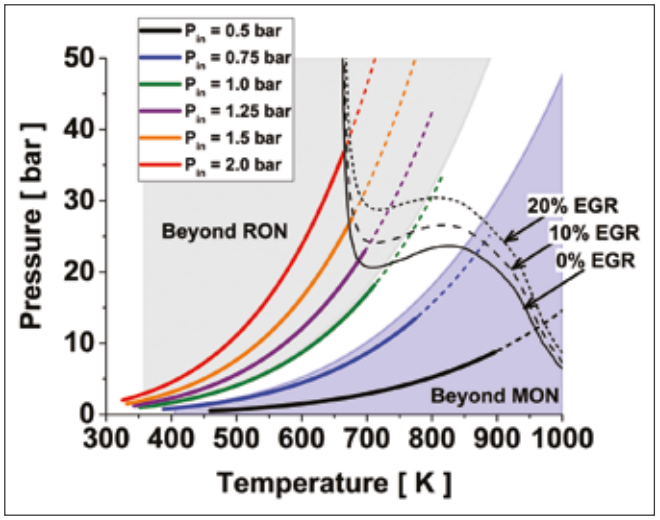


This plot of knock-limited CA50 (the crank angle at which 50% of the total heat is released) in degrees after top dead center (°CA aTDC) as a function of OI for seven widely disparate fuels shows a linear relationship independent of each fuel's chemical composition. MB = methyl butanoate. Figure by James Szybist, ORNL

Co-Optima Research Reveals Why EGR Loses Anti-Knock Effectiveness Under Boosted Conditions

Knock limits the ability to operate engines at their highest efficiency. Exhaust-gas recirculation (EGR) is effective at attenuating knock in naturally aspirated SI engines, but is much less effective in boosted engines. While EGR addition increases the compression pressure and temperature—both of which promote knock—EGR simultaneously slows the reactions that lead to knock. This effect wins out under conditions relevant to naturally aspirated engine operation.

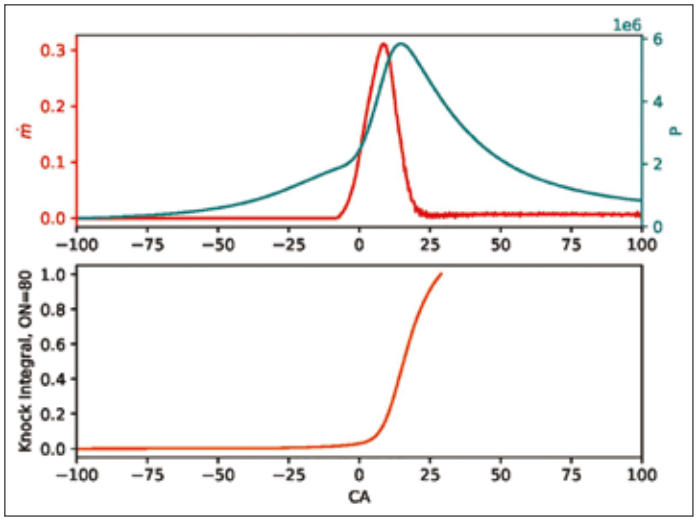
Co-Optima researchers paired experimental results with kinetic models to reveal that the influence of EGR on the reaction kinetics changes based on engine operating conditions. At intake manifold pressures of about 1.25 bar or less, EGR is highly effective at slowing the reaction rates, thereby mitigating knock. However, under more highly boosted conditions, the combustion follows different reaction pathways where EGR has less effect on the reaction rates, so EGR fails to attenuate knock. The same trend was observed for all three fuels investigated. These results aid identification of engine operating conditions under which diluents such as EGR or air can be most effective at mitigating knock, helping to identify fuel properties and engine design parameters that yield performance benefits.



Pressure vs. temperature graph for the Co-Optima alkylate fuel. Color-coded curves represent a range of intake manifold pressures; pressures greater than 1.0 bar representing boosted conditions. The overlaid 8-millisecond ignition delay contours for 0%, 10%, and 20% EGR demonstrate that at high boost conditions, EGR has little effect on ignition delay, and thus on knock propensity. Figure by James Szybist, ORNL

Ignition Delay Data Linked with Engine Knock-Integral Modeling

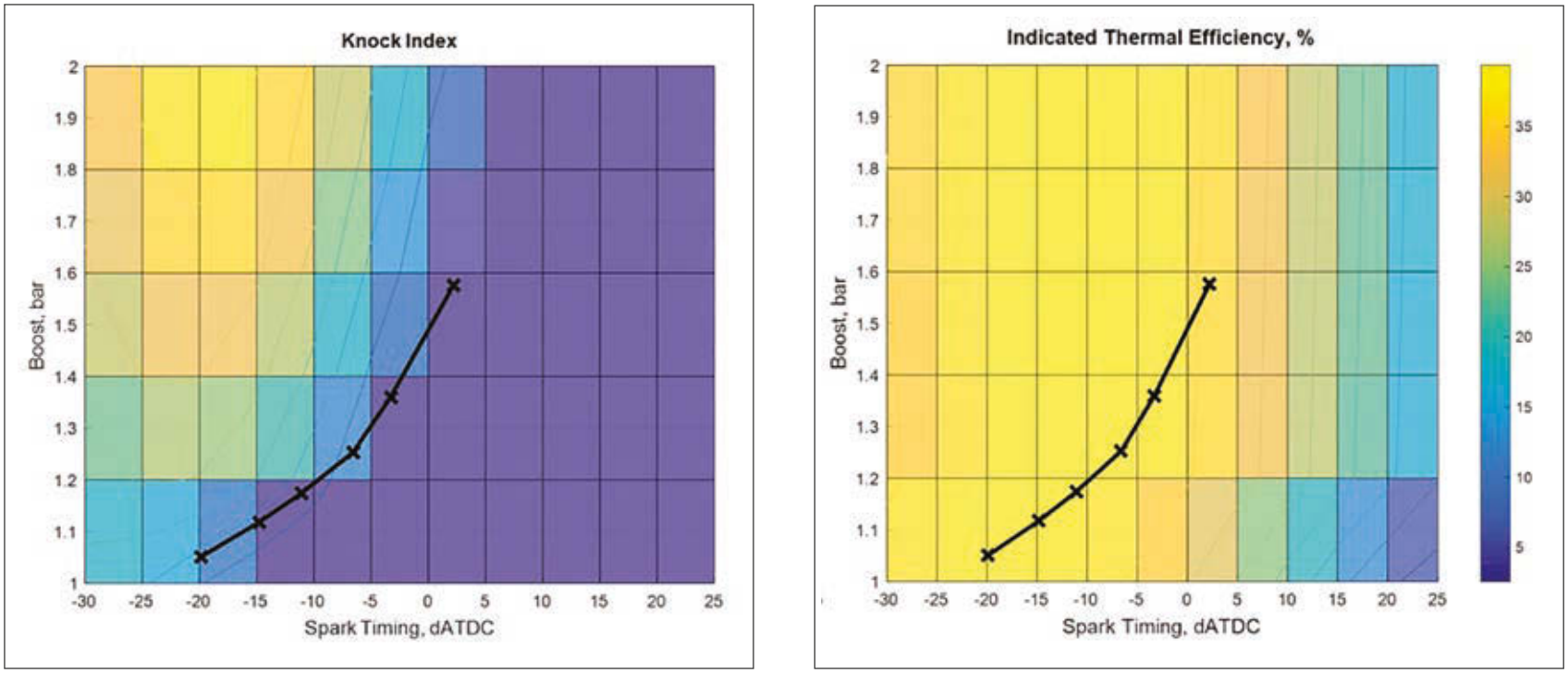
Fundamental ignition delay data across a wide range of temperatures and pressures provides invaluable insight into fuel property impacts on combustion, as well as critical data for kinetic model validation. However, there are few tools available that link these measurements directly to key engine parameters such as knock. Co-Optima researchers have developed a method for predicting knock from bench-scale ignition delay measurements for gasoline surrogates blended with oxygenated compounds and burned in a bench-scale constant volume combustion chamber (CVCC). The method involved development of a zero-dimensional, two-zone engine knock simulation that uses a knock-integral approach to calculate end-gas autoignition from CVCC ignition-delay data by feeding unburned gas thermodynamic conditions into a modified Livengood-Wu knock integral calculation and the Douaud and Eyzat correlation. The simulation provides more insight than RON, motor octane number (MON), and cetane numbers alone and can help identify approaches for optimizing engine efficiency. For example, 3-D surface maps of ignition delay at lower temperatures illustrate how spark retard can be leveraged to increase boost while avoiding knock, a relationship previously only linked to favorable reduction of MON at fixed RON.



Plots of the mass of fuel burned, cylinder pressure, and knock integral calculation for an engine simulation using bench-scale ignition delay data. The simulation predicts end-gas autoignition in the cylinder. Figure by Ray Grout, NREL

Research Evaluates Knock Limits for Candidate Fuels through Engine Simulation

Well-validated engine models can yield insights that complement those from experimental observations by simulating conditions not easily achieved in the laboratory. Co-Optima researchers used engine simulations to evaluate fuel property impacts on knock limits under engine operating conditions beyond the capabilities of experiments with fixed engine configurations. The team developed a model of the Ford 1.6-L gasoline direct injection (GDI) engine, validated it with experimental data for the Co-Optima alkylate core fuel, and used it to explore knock limits and potential performance benefits at conditions that could not be replicated with the stock engine hardware, including higher boost levels. The results show that the stock hardware is already well optimized to get maximum benefits from this fuel. Planned future efforts include adding a conjugate heat transfer model to predict surface temperatures inside the combustion chamber, evaluating other Co-Optima candidate fuel blends to determine whether those fuels may provide additional efficiency benefits by allowing operation at higher boost/compression ratio, and developing engine fueling maps over the extended speed/load range to enable fuel-economy simulations. This simulation approach provides an accurate and rapid means to identify fuel property/engine parameter combinations that yield high efficiency and can subsequently be investigated in more detail by higher fidelity simulations.



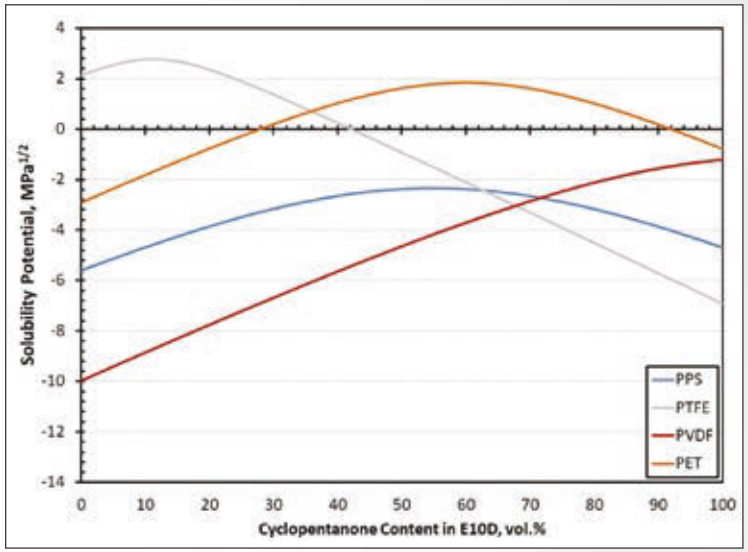
A GDI engine model developed in GT-Power® accurately predicts transition to knock and allows evaluation of knock limits beyond the capability of fixed hardware to more fully explore potential benefits of optimized designs. Results are shown for 98 RON alkylate fuel at 2000 RPM with the black line indicating experimentally observed knock-limited spark timing at the same conditions. Figure by K. Dean Edwards, ORNL

LDV Scenario Analysis Aligns Research Priorities with Highest Impacts

The most impactful innovations are born out of a clear need for technology. A light-duty scenario analysis was conducted to help identify the market needs, end-user affordability, energy choices, and barriers for fuels and vehicles that might result from Co-Optima research. These studies helped researchers align and prioritize technical targets with an eye toward maximizing impact and opportunities for large-scale implementation. Co-Optima researchers developed components of hypothetical rollout strategies for two representative boosted SI fuels—E40 (40% ethanol, 60% gasoline) and catalytic fast pyrolysis gasoline (CFPG)—at different ends of the compatibility spectrum. CFPG is readily compatible with infrastructure, while E40 is currently incompatible with the majority of vehicles and fuel retail equipment. The strategy components applicable to the modeled fuels can be extended to other Co-Optima blendstocks based on responsive fuel property traits. Results of the study support decisions on prioritization of technical targets and future research thrusts. Examples of this include trade-offs involving fuel properties, compatibility with existing infrastructure, energy and emissions profiles, and co-product production. These observations have helped guide technical team activities by helping to target blendstocks with both the optimal fuel properties and greatest potential for adoption by industry and users.

Blendstocks Analyzed for Compatibility with Fuel Systems Plastics

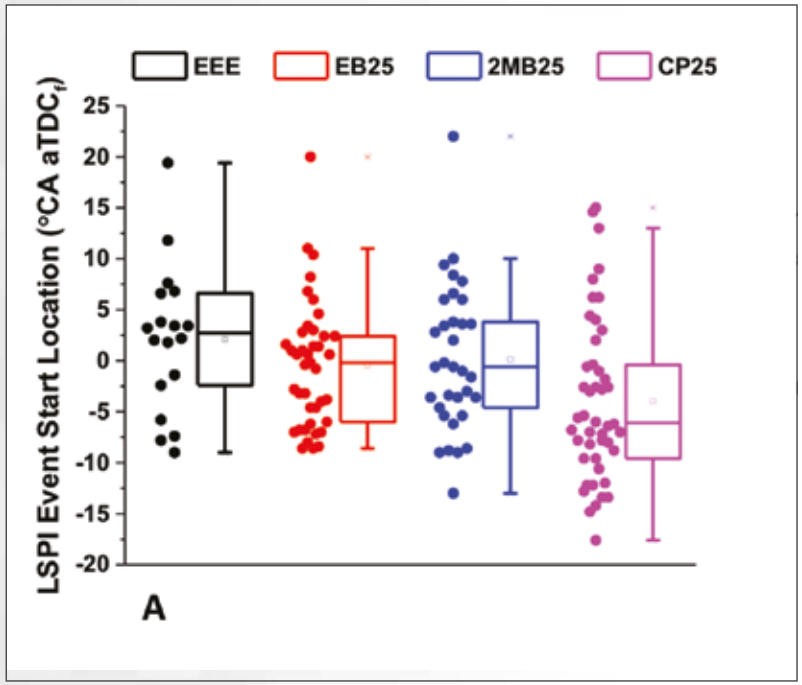
Prospective new blendstocks must be assessed for compatibility with materials—plastics, elastomers, and metals—commonly used in vehicles and infrastructure. As part of a comprehensive materials compatibility survey, Co-Optima researchers conducted a Hansen solubility analysis (a technique used to study fluid-fluid interactions) of 14 plastics commonly used in fuel systems with 39 blendstock candidates and blended fuels. This is the first study to methodically analyze the compatibility of the plastics used in fuel systems and potential new fuels. Surprisingly, in many instances the peak solubility (which indicates greater incompatibility) occurs for blended fuels rather than the blendstocks itself. The data indicate that materials such as polyphenylene sulfide (PPS), polyvinylidenefluoride (PVDF), polyethylene terephthalate (PET), nylons, acetal, polyetherimide, polyvinyl chloride, high density polyethylene, and polybutylene terephthalate will likely have no compatibility issues. However, the use of polytetrafluoroethylene (PTFE or Teflon) is unsuitable at low blend concentrations with certain blendstocks, particularly ketones. These results help identify materials requirements that may be necessary to support commercial use of new blendstocks and develop mitigation strategies, such as molecular structure modifications that increase compatibility while maintaining desired combustion properties.

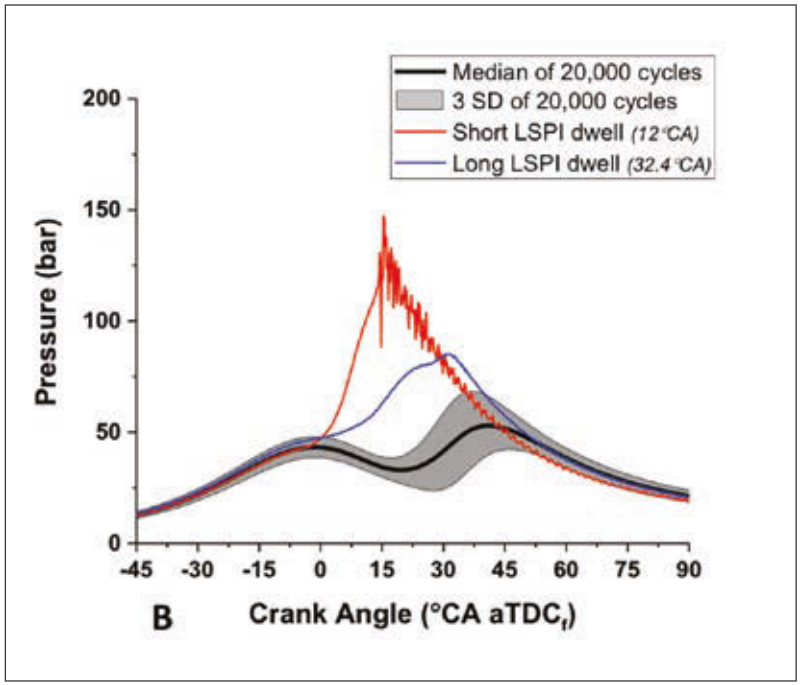


Solubility results for the majority of infrastructure and fuel system plastics show good potential compatibility with the blendstock candidates. However, solubility analysis indicated that PTFE exhibits potential incompatibility at low blend levels. This is shown in the plot for cyclopentanone, as the solubility potential exceeds 2 MPa$^{1/2}$. The line at solubility parameter = zero indicates moderate interaction between the blendstock and the plastic and values less than 0 are likely compatible. Values between 0 and 2 MPa$^{1/2}$ may be suitable depending on application. Figure by Mike Kass, ORNL

Fuel Properties Beyond Distillation Influence LSPI

Low-speed pre-ignition (LSPI) is a stochastic and rare, yet potentially highly damaging, abnormal combustion event that limits the efficiency potential of boosted SI engines. To investigate the dependence of LSPI on fuel distillation characteristics and flame speed, Co-Optima researchers examined the performance of four fuels: neat gasoline, and three fuels in which gasoline was splash-blended with 25% by mass of a ketone (cyclopentanone), an alcohol (2-methyl-1-butanol), and an aromatic (ethylbenzene). All three splash-blended fuels have similar distillation profiles but exhibit a range in molecular configuration and flame speeds. The team carried out engine experiments at identical LSPI-prone operating conditions. Findings showed that fuels with similar boiling properties and octane numbers can exhibit similar LSPI number counts, in accordance with established literature, but with vastly different LSPI magnitudes, dwells, and intensities. The results support theories that fundamental fuel properties such as flame speed are critical to characterizing a fuel's LSPI propensity and behavior, lending insight into how specific fuel properties can affect downsizing and downspeeding opportunities for fuel economy improvement.

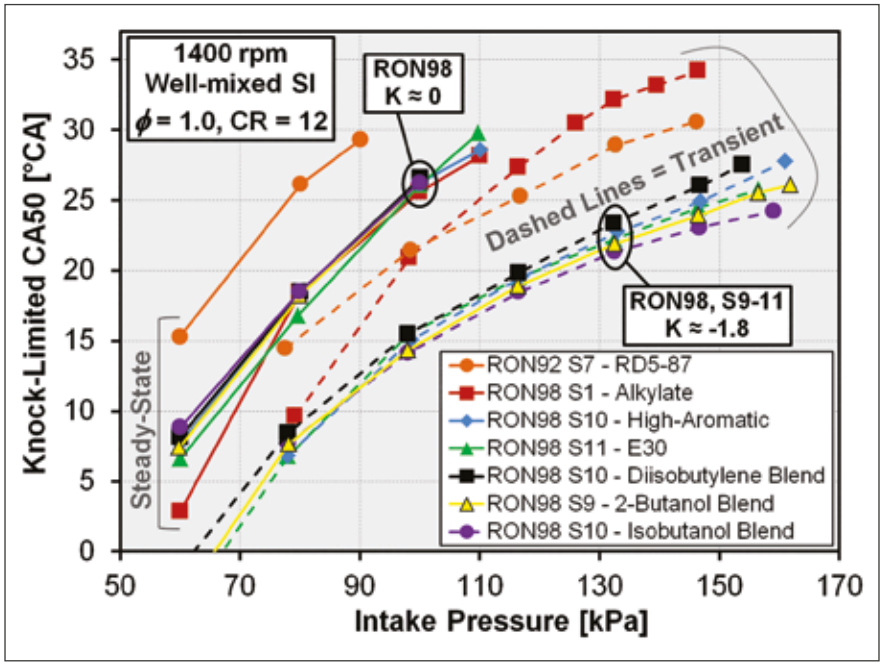




Plot A shows the starting crank angle after top dead center (aTDC) of a LSPI event for four fuels: EEE certification-grade gasoline, and EEE with 25% by mass of ethyl benzene (EB25), 2-methyl-1-butanol (2MB25), and cyclopentanone (CP25), demonstrating fuel effects on LSPI onset advance. Plot B shows the differences in LSPI event dwell with matched LSPI event starting times. Figure by Derek Splitter, ORNL

High-Sensitivity Fuels Benefit Transient SI Engine Operations, Even Under Moderate Boost

Co-Optima researchers developed a methodology to measure knock limits during engine conditions that mimic vehicle accelerations of about 20 seconds and applied it to a number of fuels including the Co-Optima RON 98 core fuels. Regular market gasoline performs worse than all RON 98 fuels under steady-state conditions. Under the cooler load-transient conditions, all fuels are less knock-limited, and the rank order of the fuels' anti-knock qualities are generally consistent with their RON and S, as evaluated within the octane index framework. These observations indicate that advanced fuel blends with high S provide superior knock suppression during vehicle acceleration, potentially offering increased performance and fuel economy.



Knock-limited combustion phasing (CA50) as a function of intake pressure, both for steady-state and load-transient operation, for fuels with a range of S. Lower values indicate higher knock resistance. RD5-87 represents regular-market gasoline. For boosted operation with Pin > 100 kPa, the best knock suppression is observed for the isobutanol blend. Figure by Magnus Sjöberg, SNL

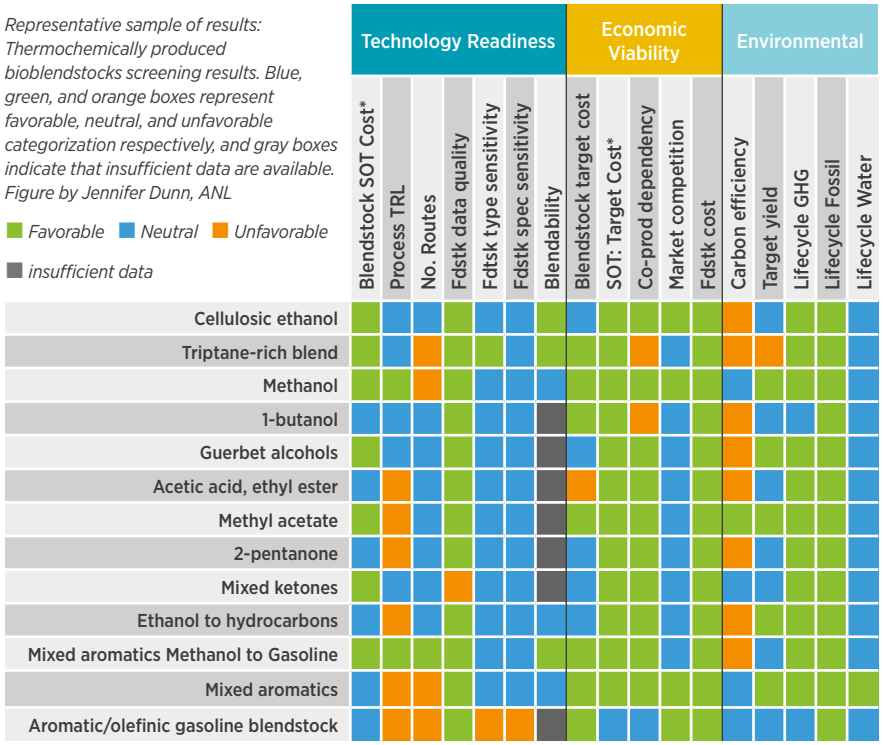
Bioblendstocks Evaluated for Near-term Economic, Scalability, Environmental Viability

Co-Optima researchers analyzed 24 blendstocks with the potential to improve boosted SI engine efficiency for their technology readiness, economic viability, and environmental performance when produced from biomass. Production processes included biochemical (fermentation), thermochemical (gasification or pyrolysis), and/or hybrid (fermentation followed by catalytic conversion) processes. To carry out the assessment, 17 metrics were developed against which each blendstock was assessed as either favorable, neutral, or unfavorable. These results help identify research challenges that need to be addressed to increase viability.

Representative sample of results: Thermochemically produced bioblendstocks screening results. Blue, green, and orange boxes represent favorable, neutral, and unfavorable categorization respectively, and gray boxes indicate that insufficient data are available. Figure by Jennifer Dunn, ANL

Favorable *Neutral* *Unfavorable*

insufficient data



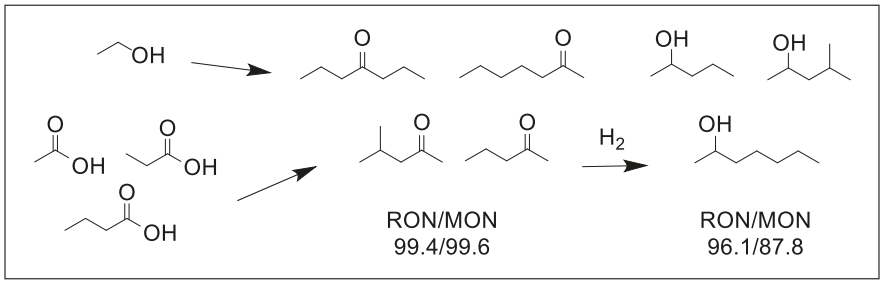
**SOT = State of Technology*

Two New Biomass Mixtures Show Excellent Potential as Blendstocks

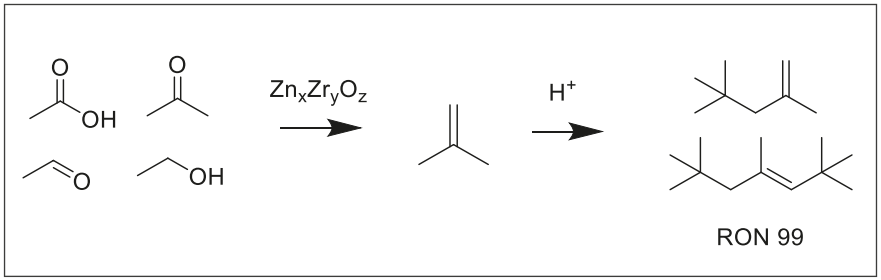
A key focus of Co-Optima research is determining how molecular structure impacts fuel properties, as this understanding forms the basis for identifying new high-potential blendstocks. Co-Optima researchers identified two mixtures—mixed ketones and an iso-olefin mixture—that are readily derived from biomass and that have properties that improve boosted SI operation. The team derived these new mixtures from feedstocks that are readily available or economically viable, increasing their feasibility of being produced through sustainable and economic manufacturing methods.

The ketone mixture was generated from alcohols, such as ethanol, or from volatile fatty acids (Scheme 1). The mixed ketones have about 30% higher energy density compared to ethanol and boil over a wide range. They also exhibit a RON of 99 (regular gasoline is 91–92). This research provides a means to modify RON, S, and energy density for a variety of oxygenated blendstocks and the mixtures may be converted to higher alcohols with greater octane sensitivity, providing a "lever" to co-optimize this fuel blendstock with advanced engine architectures to improve fuel economy.

The iso-olefin blendstock was produced from a mixture of aqueous oxygenates that are not suitable as fuel blendstocks (Scheme 2). The iso-olefin mixture has a RON estimated at 99 via ignition quality testing, has lower vapor pressure than many olefins in current market gasoline, and should be fully compatible with current fuel delivery and vehicle infrastructure. In addition to identifying new promising blendstocks, these results highlight the importance of utilizing structure-property relationships to guide identification of new high-value blendstocks.



Scheme 1: Mixed ketones were produced from lower molecular weight alcohols or acids. The mixed ketones may also be reduced to alcohols.



Scheme 2: Iso-olefins were produced through an isobutene intermediate from aqueous oxygenates over a zinc/zirconia catalyst. Figures by Karl Albrecht, PNNL

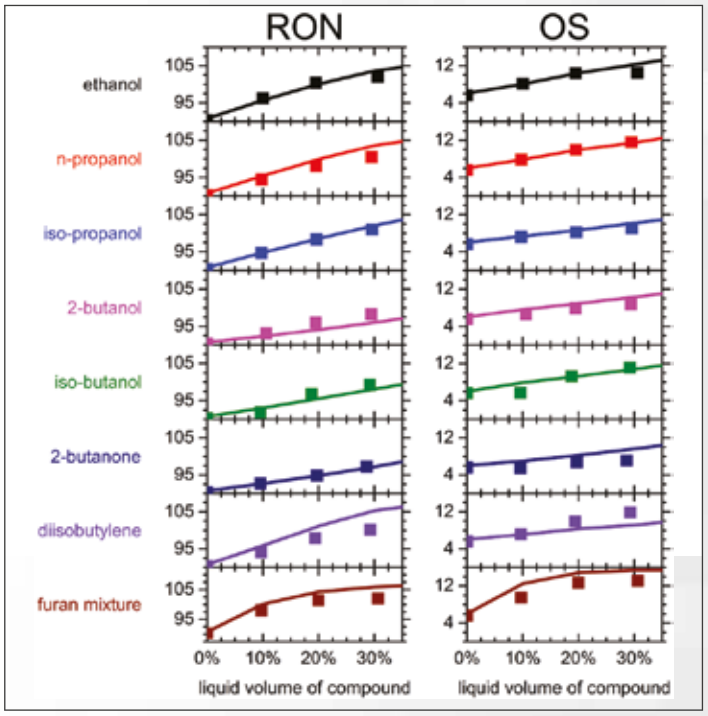
Gum Formation Mechanism Determined for High-Octane Alkyl Furans

Co-Optima researchers found that a blendstock comprised of methyl and dimethyl furan provides higher blending RON and S than the other boosted SI blendstocks studied. However, oxidation studies show that the furans lead to gum formation 10 times higher than the level observed for commercial fuels, potentially gumming up a vehicle's fuel supply systems. Since the furans can be produced readily from biomass and impart such high RON and S, Co-Optima researchers are interested in finding a solution to excess gum formation. Conventional gasoline antioxidants are only mildly effective at slowing this reaction. The team conducted an experimental and theoretical study of the liquid-phase oxidation mechanism to understand the fundamental underlying chemical mechanism responsible for gum formation and potential routes to mitigate this issue. Reaction pathways derived from quantum chemical calculations identified the gum formation mechanism, which is different from those exhibited by di-olefins and biodiesel, explaining why conventional antioxidants have limited effectiveness. The understanding developed from this work will help industry to identify chemical additives that can reduce or mitigate gum formation from furan-containing fuels, increasing the commercial viability of this blendstock.

Gum produced after 24 hr at 100°C under 700 kPa O2 initial oxygen pressure (ASTM D873 method) for 10 vol% blend of dimethyl furan in iso-octane. Photo by Robert McCormick, NREL

Chemical Kinetic Model Predicts Octane Blending for Co-Optima Blendstocks in Gasoline

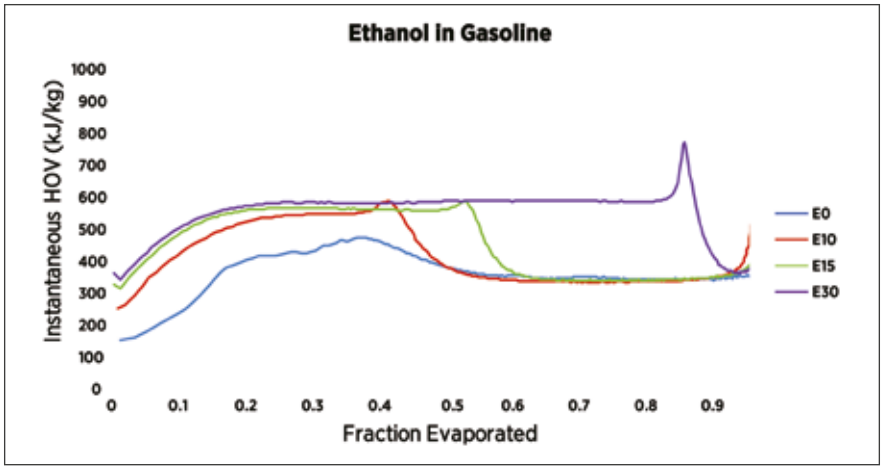
Accurately predicting the octane blending behavior of blendstocks in gasoline from fundamental kinetic principles is essential for conducting accurate simulations of engine performance, yet this ability has remained an elusive challenge for half a century. Co-Optima researchers developed a chemical kinetic model that reproduces the measured octane blending behavior of blendstocks in a base gasoline with good accuracy. The demonstrated ability of the chemical kinetic model to simulate octane blending behavior and reproduce data from other fundamental combustion experiments gives Co-Optima researchers confidence in using the model for predicting and providing understanding of combustion behavior in boosted, downsized SI engines.



The predictions of octane blending of Co-Optima blendstocks in a 4-component base gasoline using the Co-Optima chemical kinetic model (curves) compared to experimentally measured RON and S [symbols]. Figure by Bill Pitz, LLNL

Improved DSC/TGA Method Evaluates Gasoline-Ethanol Blend Evaporation

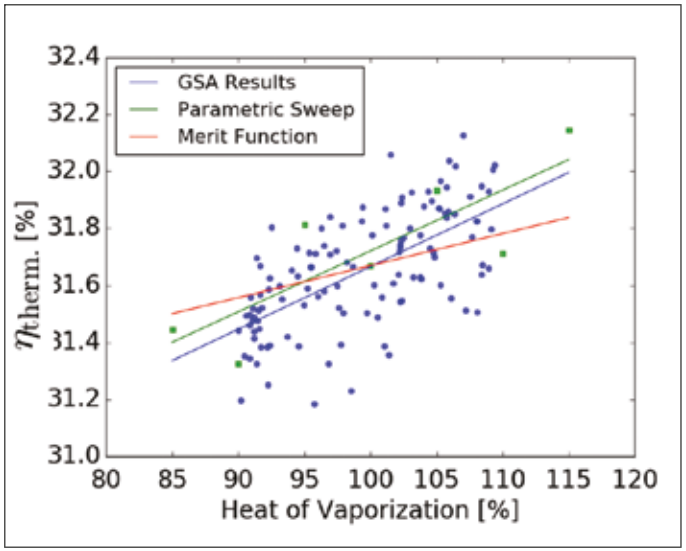
The heat of vaporization (HOV) of a fuel has been shown to impact boosted SI engine performance, yet there are few experimental techniques that allow detailed, instantaneous HOV measurements of real complex fuels that can help interpret results from boosted SI engine experiments. Blending polar oxygenates such as low molecular weight alcohols into gasoline can provide an evaporative cooling effect in direct-injection (DI) engines that increases the fuel's knock resistance. This cooling arises from the larger HOV of these blendstocks compared to hydrocarbons. Co-Optima researchers developed a differential scanning calorimetry (DSC)/thermogravimetric analysis (TGA) method to investigate the effect of oxygenates, such as alcohols, on the instantaneous HOV of gasoline-oxygenate blends. These data are important for validating droplet evaporation models and providing new insights into composition stratification due to the fuel evaporation process within engines. Experiments with ethanol have shown that increasing the amount of ethanol initially increases the overall HOV of the sample, but that the instantaneous HOV drops off significantly once the ethanol has evaporated at fractions much higher than the ethanol concentration. The team believes it is the first to apply this methodology to complex gasoline-ethanol mixtures.



Comparison of the instantaneous HOV of gasoline-ethanol blends from 0% to 30% ethanol versus the fraction of sample evaporated. The addition of ethanol shows an increase in the instantaneous HOV as well as an extension of the increased HOV plateau as more ethanol is blended into the sample. Figure by Gina Fioroni, NREL

First Global Sensitivity Analysis Reveals Insights of Fuel Properties on Engine Performance

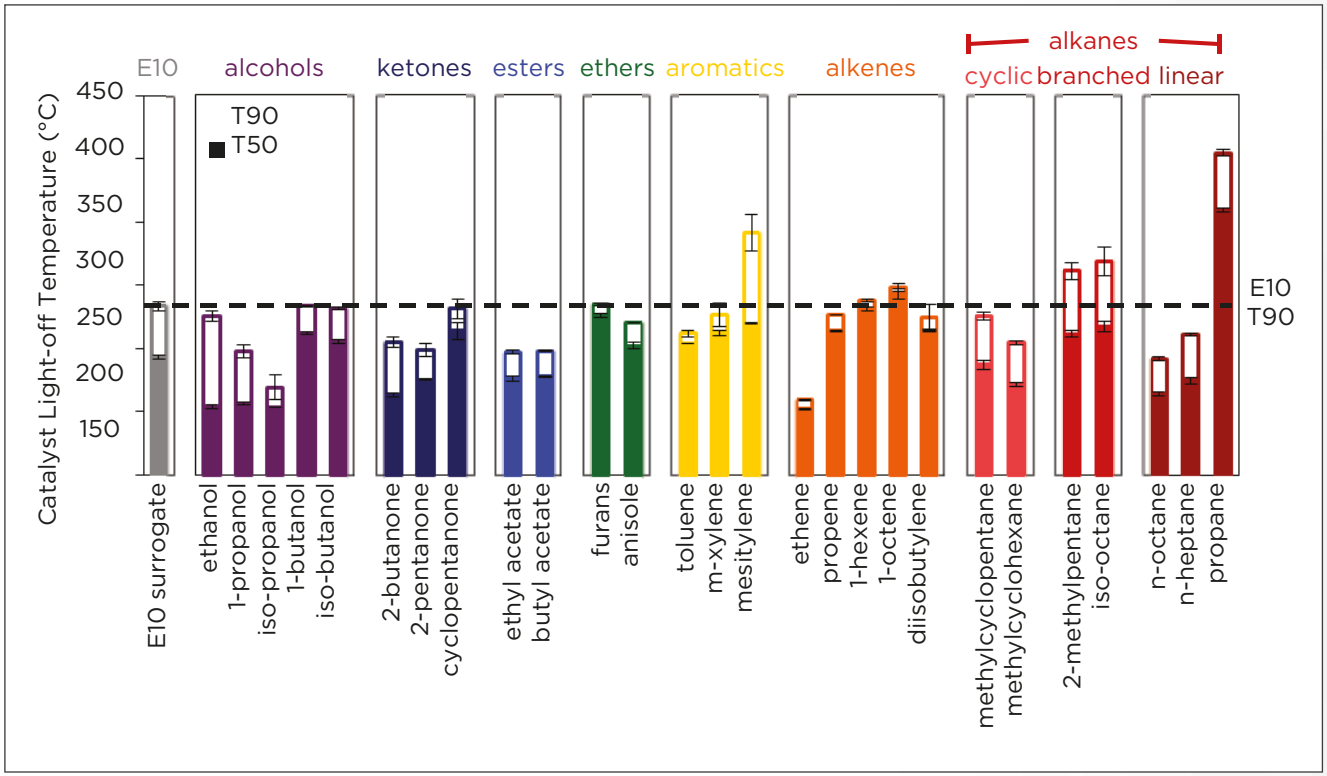
A major advantage of engine simulations is that the fuel properties can be varied completely independently of each other, which is difficult or impossible to do experimentally. A global sensitivity analysis of fuel properties on engine performance was performed to better understand the importance of fuel properties not included in the boosted SI merit function on engine efficiency. Six different fuel physical properties (viscosity, surface tension, HOV, vapor pressure, density, and specific heat) were varied across 120 total simulations. Of these six properties, only HOV is currently included in the merit function and is included as a tie point. The engine platform and operating condition were representative of well-mixed SI engines. Results showed that of the fuel properties evaluated, HOV has the most influence on engine thermal efficiency, and the effect was more than expected from merit function predictions. The results confirmed that HOV has a significant effect even when varied independently of fuel composition which is only possible in simulations, and other fuel physical properties have much smaller effects. Current efforts are focused on determining the significance of the differences between simulation and merit function HOV coefficients.



Scatter plot of engine thermal efficiency vs. a fuel's HOV (as percentage of the baseline) for global sensitivity analysis simulations where six fuel properties including HOV were independently randomly perturbed. The simulation-derived slopes (blue and green lines) are greater than expected from experiments (red line). Figure by Noah Van Dam, ANL

New Term in Co-Optima Boosted SI Merit Function Accounts for Efficiency Impact of Cold-Start Emissions

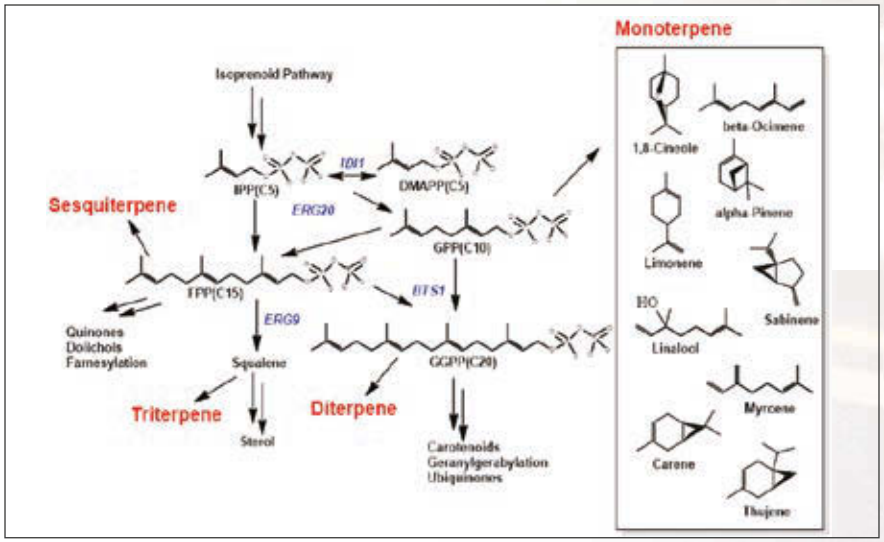
Commercial high-efficiency engines must meet emissions regulations, and need to accommodate changes in emission profiles due to fuel composition variations. Co-Optima researchers are investigating the impact of potential new blendstocks on emissions control systems to identify potential benefits or concerns. As part of this effort, researchers developed an emissions control term for the Co-Optima boosted SI merit function based on the fuel penalty associated with catalyst heating during cold start. The team then measured the catalytic light-off temperatures needed to evaluate the merit function emissions control term for more than 30 molecules and mixtures, including a wide range of Co-Optima blendstock candidates and conventional petroleum-derived fuel components. The catalytic light-off investigations showed that most of the oxygen-containing blendstock candidates had relatively low light-off temperatures. The catalytic reactivity of blendstocks that did not contain oxygen was highly dependent on the molecular structure in sometimes unexpected ways: branched alkenes were more reactive than linear alkenes, while branched alkanes were much less reactive than linear alkanes, for example. The merit function emissions control term and associated fuel property measurements provide a method for quantifying the potential impacts of fuel composition changes on the emissions control of nitrogen oxides, non-methane organic gases, and carbon monoxide. This approach explicitly includes emissions control impacts when co-optimizing fuels and engines.



Temperatures at which 90% (T90) and 50% (T50) hydrocarbon conversion occurs over an aged commercial three-way catalyst in a synthetic exhaust mixture containing the organic species listed. The T90s for the single-component blendstocks provide a basis for estimating T90s for fuel blends, yielding the emissions control term for the Co-Optima boosted SI core merit function for each fuel blend. For reference, the dashed line indicates the T90 for E10 (a blend of 10% ethanol and 90% gasoline). Figure by Josh Pihl, ORNL

Biosynthesis of Monoterpenes Produces Novel Blendstock Candidates

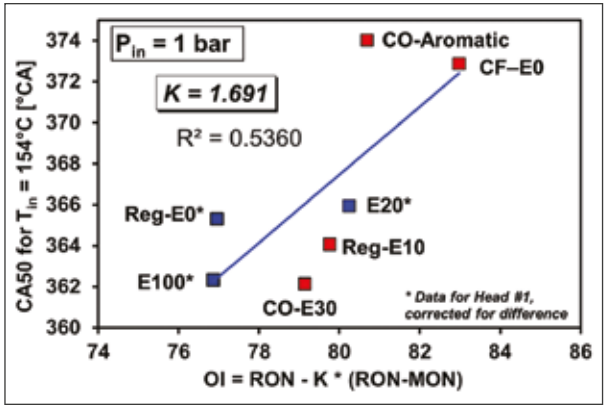
Co-Optima research has shown that higher olefins contribute desirable boosted SI properties such as high RON and S, particularly if the structures contain branching and/or strained rings. Monoterpenes, a class of olefins that contain these functional groups, are potentially promising blendstocks. To assess this potential, Co-Optima researchers identified several monoterpenes predicted to have high RON and high energy density as candidates for boosted SI blendstocks. To demonstrate the feasibility of producing these molecules biologically, genes encoding 16 terpene synthases covering nine different monoterpenes were engineered into a yeast, and the researchers demonstrated the successful production of six monoterpenes. Of those six, 1,8-cineole was produced at the highest titers and its production from a cellulose stream was subsequently demonstrated. The fuel properties of cineole were examined in more detail, and it was determined to have a RON of 99 and 1.65 times the energy density of ethanol. Based on these promising initial results, additional studies are underway to assess the performance of cineole and other related terpenes against other key fuel properties.



Terpene Biosynthetic Pathway: A yeast was engineered to produce several monoterpenes with potential to be used as high RON bioblendstocks or as gasoline blendstock for oxygenated blending replacements. Figure by John Gladden, SNL

Conventional Autoignition Metrics Fall Short for Naturally Aspirated and Boosted Low Temperature Gasoline Combustion Engines

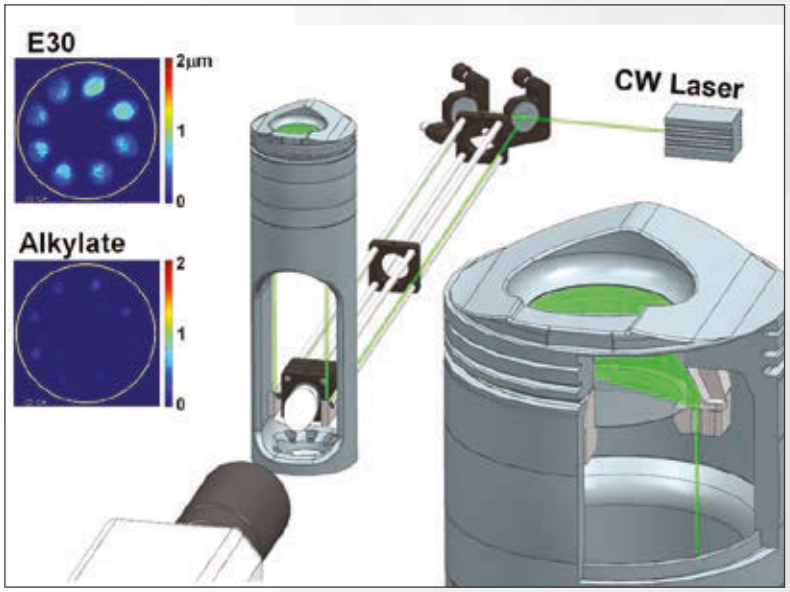
Low-temperature gasoline combustion (LTGC) is an ACI approach that relies on fuel autoignition rather than a spark to initiate combustion. LTGC provides high efficiency and low emissions at part load conditions, making it a promising approach for multimode operation. However, understanding how fuel properties governing LTGC operation is much less established than it is for boosted SI. Co-Optima researchers evaluated the autoignition reactivities of the Co-Optima aromatic and E30 core fuels (both with RON 98 and S~10-11) in an LTGC engine and compared them with E10 and other gasoline blends for both naturally aspirated and boosted intake pressures. The figure shows that the OI index and K factor are not sufficient for correlating the differences in autoignition reactivity of these fuels for naturally aspirated LTGC operation, even when accounting for the greater HOV of E30. The E30 core fuel is consistently more reactive than the high-aromatic core fuel under boosted conditions despite these two fuels having nearly identical RONs and MONs, indicating that RON, MON, and OI index are not sufficient to describe the critical fuel properties governing LTGC operation. Current efforts are investigating the extent to which including phi sensitivity—the sensitivity of the autoignition reactions to the local equivalence ratio in the charge—improves the correlation with combustion phasing. Experiments have shown that phi sensitivity combined with appropriate partial fuel stratification can be used to control the heat release rate to reduce noise and knock propensity.



OI vs CA50 for the Co-Optima E30 (CO-E30), high-aromatic (CO-Aromatic), and other fuels. The correlation is poor with an R2 of only 0.536. Adjusting the E30 point to compensate for its higher HOV gives only a modest improvement, R2 = 0.596 (not shown). Figure by John Dec, SNL

Optical Diagnostics Quantify Wall Wetting and Pool Fires in Direct-Injection SI Engines

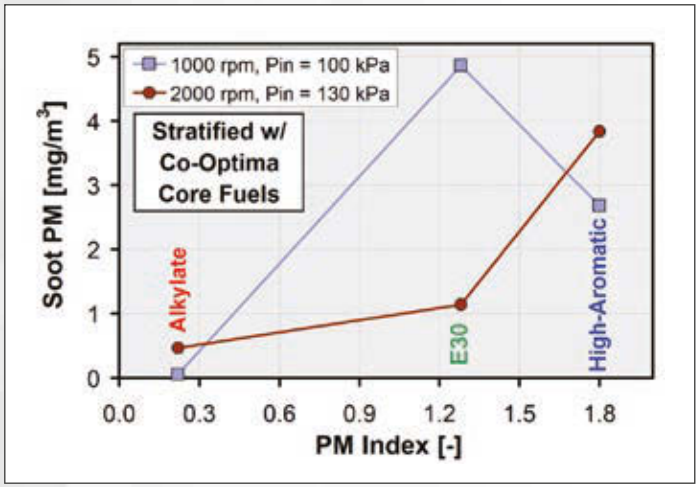
To comply with stringent exhaust emissions requirements, it is important to minimize the emissions out of an engine. The interaction of fuel sprays and piston surfaces can be problematic for some combinations of fuels and operating points, causing soot formation. To identify sources of exhaust smoke, researchers developed optical diagnostics in a direct-injection SI engine to quantify both wall wetting and pool fires. As demonstrated by the figure, the contrast between the wall films seen for the Co-Optima core E30 and alkylate fuels provide a good example of the strong effect of fuel properties on the tendency to form fuel films. These data are proving valuable in model validation as well as in providing insight into fuel injection strategies that help minimize pollutant formation.



Laser-based measurements allow the detection of fuel wall films for various combinations of fuels and operating conditions that are prone to pool fires. Figure by Magnus Sjöberg, SNL

Formation of Pool Fires Increases Engine-Out Soot Production

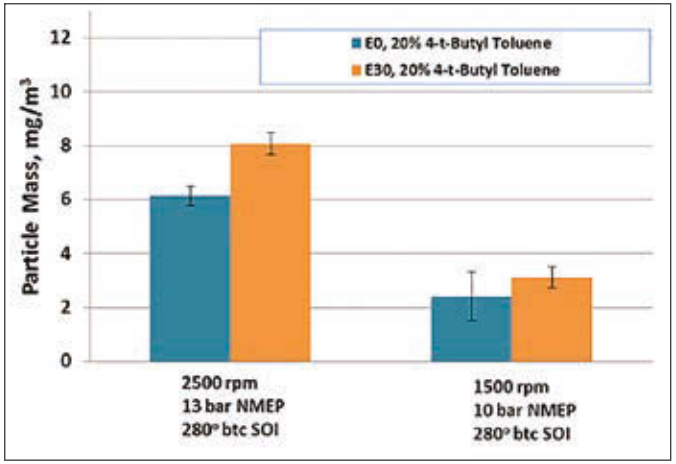
Spray-guided stratified-charge SI operation is one approach to lean, high-thermal-efficiency engines, but fuel stratification can cause high engine-out smoke levels. Operating more efficient engines requires an understanding of soot-formation pathways and how they are affected by fuel composition and fuel specifications. Combined exhaust emissions measurements and in-cylinder optical diagnostics have revealed that the enhanced vaporization cooling associated with the ethanol fraction in E30 can cause wall wetting and pool fires. For such conditions, the engine-out soot becomes higher than expected from the fuel's particulate matter (PM) index. These findings highlight both the need to further develop fuel-specification metrics that address engine PM emissions, and also to closely monitor the formation of fuel wall films for advanced combustion systems.



For boosted, stratified-charge, direct-injection SI operation at 2,000 rpm, engine-out soot increases monotonically with the fuels' PM index, as the soot formation is primarily occurring in the bulk gases. But for naturally aspirated operation at 1,000 rpm, soot emissions for E30 are higher than predicted from the PM index due to the formation of pool fires. Figure by Magnus Sjöberg, SNL

Ethanol and Aromatics Have Competing Effects on Gasoline Particle Emissions

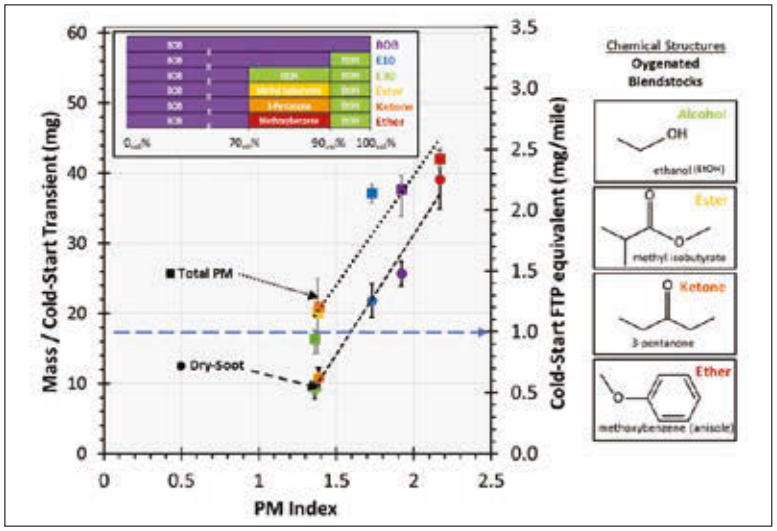
Co-Optima research has shown that alcohols and aromatics are promising boosted SI blendstocks, but data suggest that under certain engine operating conditions these blendstocks may interact and contribute to increased particle emissions. To investigate, researchers employed a direct-injection, SI, single-cylinder engine to compare fuels with and without ethanol at constant aromatic content of 20%, while varying the aromatic boiling point and vapor pressure. Results show that at high engine speed, gasoline containing ethanol and high-boiling-point aromatic compounds can produce significantly higher PM emissions relative to the no-ethanol case at constant aromatic content. This effect is not evident at slower engine speeds. Increased emissions in the presence of ethanol at higher engine speeds may be caused by the greater evaporative cooling that occurs for ethanol blends, lowering in-cylinder temperature and slowing evaporation of the heaviest gasoline components. Alternatively, non-ideal vapor-liquid equilibrium effects may retard evaporation of aromatics, leaving less time for mixing with air. These results show that match blending to keep aromatics constant—rather than allowing ethanol to dilute the aromatics—can lead to increased aromatics emissions from the aromatic compounds. These findings have important implications for blending commercial fuels that meet air quality requirements.



PM emissions from a single cylinder, direct-injection, SI engine burning E0 (gasoline with no ethanol) and E30. Both blends contained 20% by volume of the high-boiling-point aromatic compound t-butyl toluene. The chart shows that at 2,500 rpm, blending of ethanol significantly increased PM emissions, while at slower engine speeds this effect is not evident, helping to identify those conditions where ethanol has the greatest impact on PM emissions. Figure by Robert McCormick, NREL

GDI Engine Cold-Start Study Finds Oxygenated Fuel Blends May Not Be Enough to Meet Future PM Emission Targets

Fuel properties have a significant impact on both the quantity and composition of PM produced during the cold-start of GDI engines. Co-Optima researchers measured cold-start PM production with a variety of oxygenated fuel blends and non-oxygenated fuel blends (blendstock for oxygenated blending or BOB) for comparison. The results indicate that the PM index remains a valid approach for predicting the PM mass trend under cold-start conditions. The semi-volatile contribution to total PM mass was significant for all fuels studied, regardless of oxygenate content. While almost all of the oxygenated blends produced less total PM mass than the BOB, all fuels tested will have a hard time meeting the California Air Resources Board PM target of 1 mg/mile, due to the PM mass already being at or above the target in the 90-second cold start. This result suggests that oxygenate fuel blending, even up to E30, will not be enough to meet future PM emission regulations without implementation of additional measures.



Six fuels, including a BOB (which is primarily gasoline) and five oxygenate blends, were tested for PM mass emissions in a GDI engine. All five fuels were at or above the California Air Resources Board's 1 mg/mile gravimetric mass target (blue dashed line) for the Federal Test Procedure (FTP) combined cold- and hot-start cycle during the 90-second cold-start transient. The difference in the graph's two-plot series, total PM and dry-soot, indicates the amount of semi-volatile PM mass that was counted in a gravimetric mass measurement (total PM, squares), but not measured by an online micro soot sensor (dry-soot, circles). The inset illustrates the volumetric compositions of the six fuels tested and provides a color code for fuel data. Figure by Melanie Moses-DeBusk, ORNL

Three Core Fuels Produce Low Particulate Emissions with Compression Ignition Gasoline Engines

Gasoline compression ignition (GCI) is a promising ACI approach to achieving high efficiency and low emissions, but fuel property impacts on efficiency and emissions need to be better understood. Researchers tested three Co-Optima core matrix fuels—a blend of alkylates, a blend high in aromatics, and E30—for soot formation in an engine operating in a GCI mode. All fuels have a RON of 98 and the engine was operated at loads having a brake mean effective pressure between 3 and 6 bar (low/part load conditions). Combustion phasing (CA50) was held constant and EGR was swept across its entire operating range. The engine's filter smoke numbers were below 0.1 under all the test conditions, indicating that very low engine-out soot levels can be achieved with diverse fuels under GCI operation. While E30 produced the lowest engine-out soot emissions under all conditions, it also produced the highest amount of in-cylinder soot radiation. This result implies that soot can be formed in-cylinder under more stratified conditions and not result in significant soot leaving the cylinder under controlled conditions. In the case of E30, the short duration of the in-cylinder soot luminosity peaks suggests that in-cylinder soot may be quickly oxidized by the combustion reaction, resulting in low engine smoke. These results provide valuable insight into how fuel properties impact emissions for GCI and help assess its potential as a factor in achieving high efficiency and low emissions.

Technology Readiness	
Engine Speed (RPM)	**1,000**
Engine Load (bar BMEP)	**5**
EGR [%]	**20**
SOI of Main	**Adjusted for constant combustion phasing**
Boost Pressure (bar)	**1.4**
Intake Air Temp [°C]	**55**
Global λ (= 1/Φ)	**1.8**

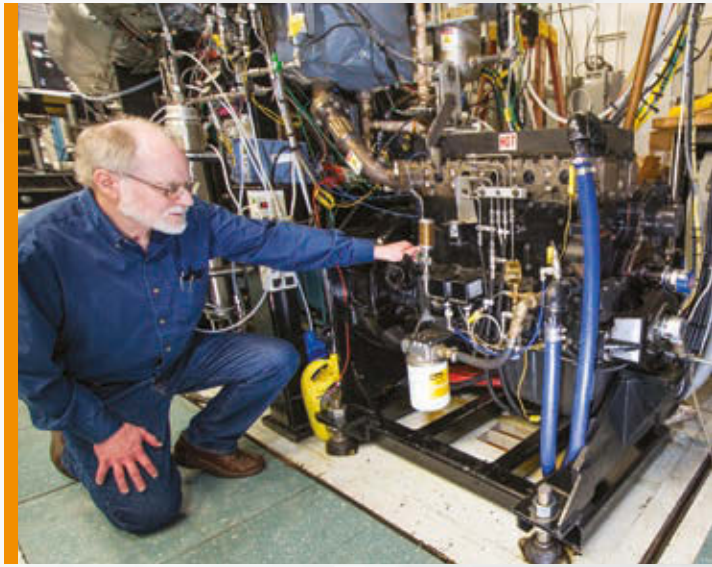
MEDIUM- & HEAVY-DUTY VEHICLE RESEARCH

Co-Optima research is targeting solutions that will impact the entire on-road fleet, including technologies needed to achieve optimal medium-duty vehicle (MDV) and heavy-duty vehicle (HDV) performance balanced with lower emissions. MDV and HDV projects range from mixing-controlled compression ignition (MCCI) to kinetically-controlled advanced compression ignition (ACI) concepts.

MCCI combustion technology is used in today's commercially available diesel engines. These engines provide high efficiency, but require sophisticated and costly emissions control technologies. Co-Optima research is examining fuel properties that can maintain engine efficiency and fuel energy density while reducing emissions and expenses.

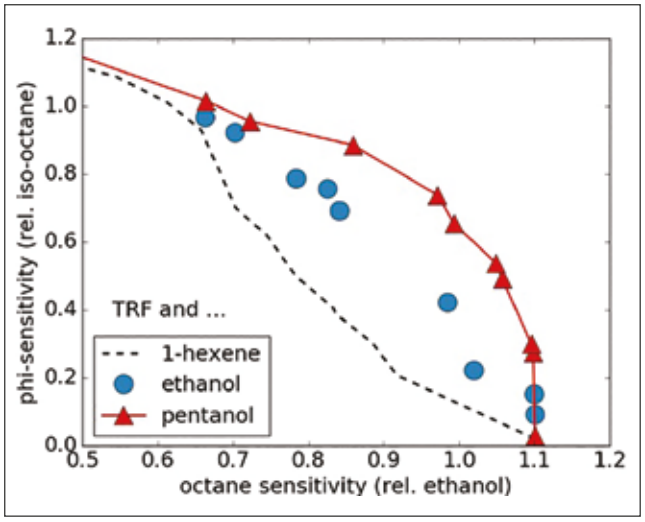
Kinetically-controlled combustion approaches hold the promise of achieving very high thermodynamic efficiencies while simultaneously yielding lower emissions. The key challenges associated with ACI engines are ensuring stable combustion over a wide speed/load range, controlling emissions despite low exhaust temperature, and providing high power density. Co-Optima MDV and HDV engine research is exploring a number of promising kinetically-controlled ACI approaches.

The following highlights provide more detail on initial accomplishments related to MDVs and HDVs.



Automated Computer Search of Phi Sensitivity Identifies Blendstocks With Potential to Improve Control of Partially Stratified Compression Ignition Engines

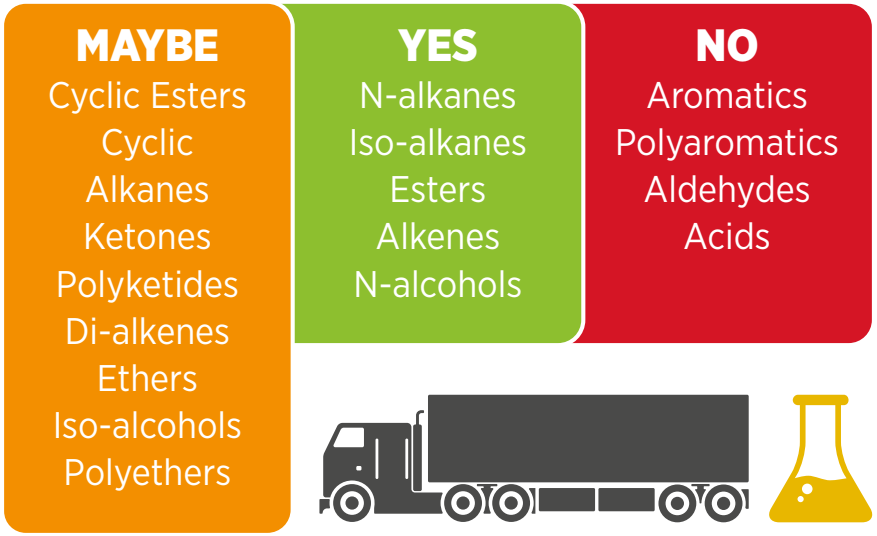
While ACI engines have demonstrated the potential to provide high efficiency and low emissions, current fuels only allow ACI operation over a small range of speeds and loads. Efforts to identify fuel properties that correlate with ACI operating range have met with limited success, as the properties commonly used for spark- and compression-ignition (CI) engines only partially correlate with ACI operability. Researchers have identified a phi sensitivity metric that correlates with a fuel's ability to improve control of a partially stratified CI engine. The new metric was combined with model-based correlations for research octane number (RON) and motor octane number (MON) using the Co-Optima gasoline chemistry model to search for blends that deliver both high phi sensitivity (better control) and high octane sensitivity (low ignition pressure sensitivity, which provides increased operating range). An initial search of more than 150,000 fuel blends uncovered blendstock combinations that provide the desired combination of these two properties. The next step will be to validate the results of this study in an engine and determine the extent to which phi and octane sensitivity explains the key features of ACI engine operability. Studies are also planned to establish the molecular basis for increased phi sensitivity.



Plot of phi sensitivity vs. octane sensitivity for blends of three components with toluene reference fuel (TRF, a gasoline surrogate). Relative to ethanol, 1-pentanol blended fuels show superior phi sensitivities at high octane sensitivities. Interestingly 1-hexene, which has the highest phi sensitivity as a pure component, does not impart high phi sensitivity when blended in surrogate gasoline. Figure by Matthew McNenly, LLNL

Functional Group Analysis Focuses Search Space for Mixing-Controlled Compression Ignition Blendstocks

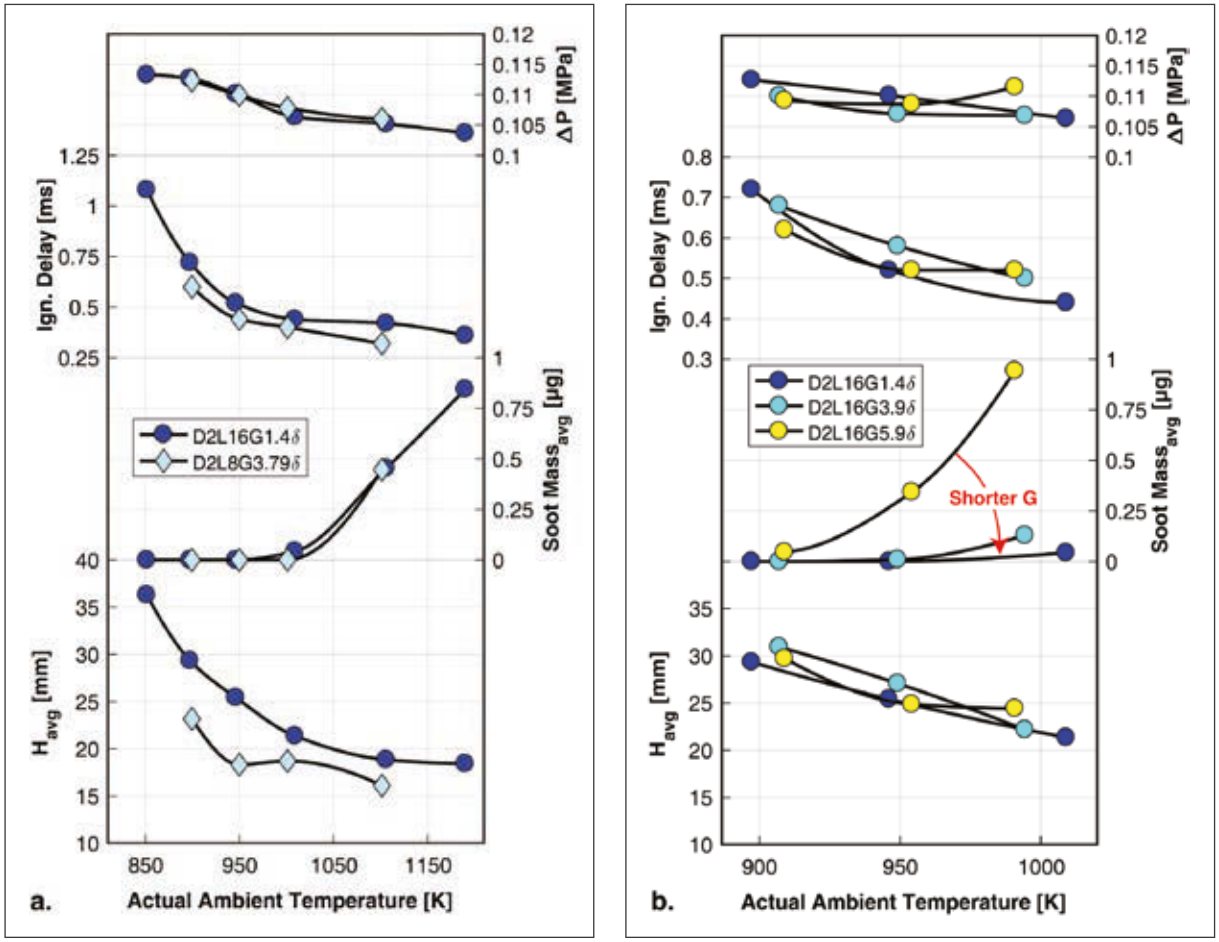
Previous studies have shown that certain classes of blendstocks can dramatically reduce engine-out particulate matter (PM) emissions from MCCI engines. Co-Optima researchers completed a systematic assessment of the suitability of hydrocarbon and oxygenate functional groups for use as a diesel-like blendstock in an advanced MCCI engine. The functional groups examined are all potentially derived from biomass and representative of a diverse range of structures and chemical reactivity. Results show that esters, alkanes, alkenes, and higher normal alcohols have properties that make them promising MCCI blendstocks, including low soot formation tendency, high cetane number, good cold flow properties, and suitable distillation properties. These results will narrow the search space for blendstocks that, when blended with petroleum-based fuels, can reduce PM emissions while maintaining high efficiency.



The suitability of compounds from a wide variety of chemical families has been evaluated for use as MCCI blendstocks. Five functional groups have been identified that can meet all requirements, while eight others may be suitable. Figure by Loren Stacks, SNL

Research Demonstrates Ducted Fuel Injection Assemblies Can Be Shortened by Half

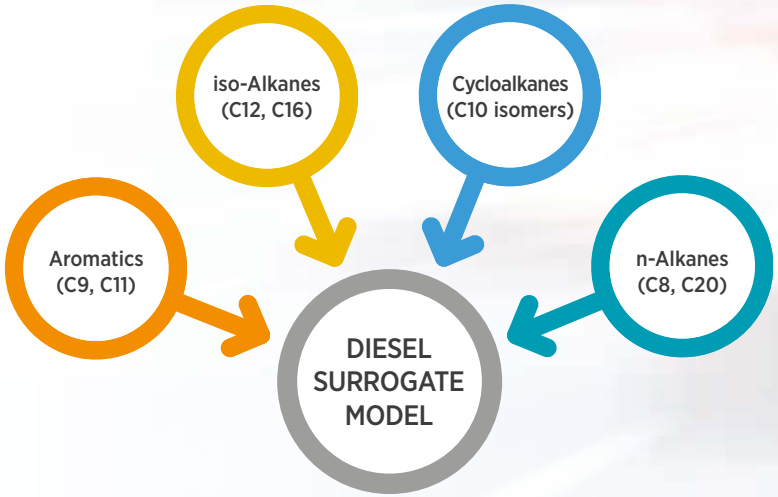
Ducted fuel injection (DFI) is a new approach to MCCI that dramatically changes the physics of in-cylinder fuel-air mixing and has shown the potential to improve the engine-out emissions and efficiencies of CI engines. Co-Optima researchers demonstrated that the dramatic soot-attenuation potential of a 2-mm-diameter duct is not significantly affected by shortening its length from 16mm to 8 mm, and that performance is significantly improved by shortening the standoff distance between the injector orifice exit and the duct inlet plane from 5.9 mm to 1.4 mm. Although the reasons for these early observations are not yet well understood, the former result may be caused by diminishing returns from extending the duct length beyond a certain point required for sufficient local mixing enhancement. The latter result may be caused by a shorter standoff distance that allows only the cooler, denser gases in the boundary layer near the vessel wall to be drawn into the duct. Regardless of the underlying mechanisms, these results indicate that the overall length of the DFI assembly can be cut in half while maintaining or improving performance, which would make it much simpler to avoid interferences between the ducts and the moving valves and pistons of the engine. These results help establish the fundamental principles of DFI operation and will guide experiments aimed at assessing the maximum benefits achievable with this new combustion approach.



Recent parametric studies indicate the potential for shortening overall duct-assembly length while maintaining or improving performance. All results are for ducts with a 2-mm inside diameter. Duct length is denoted by L and standoff distance by G. a. Shortening L from 16 mm to 8 mm does not have a detrimental effect on soot mass. b. Decreasing G from 5.9 mm to 1.4 mm lowers the soot mass for duct with L = 16 mm. Effects on the flame liftoff length (Havg), ignition delay, and total vessel pressure rise (ΔP) are also shown for reference. Figure by Ryan Gehmlich and Charles Mueller, SNL

Surrogate Kinetic Model Simulates the Behavior of Diesel Fuels

Surrogate fuels are blends of a small number of molecules that match specific physical or combustion properties of more complex fuels, such as petroleum-derived fuels that typically contain hundreds or thousands of individual components. Kinetic models of surrogate fuels allow the reactivity of real fuel to be simulated in a computationally tractable manner. A detailed chemical kinetic surrogate model was developed by Co-Optima researchers to represent the base diesel fuel that will be used to evaluate blendstocks for use in medium- and heavy-duty applications. Petroleum-derived diesel fuel has previously been represented in kinetic models by one or two components—too few to represent all the major chemical classes in diesel fuel. For the first time, a detailed kinetic model has been developed with components to represent all the major chemical classes in diesel fuel: single- and multi-ring aromatics; naphtho-aromatics; and n-, iso-, and cycloalkanes. The model was validated using experimental data on ignition delay times from shock tubes and rapid compression machines over a wide range of temperature, pressure, and fuel/air equivalence ratio. With this model, the combustion behavior of the base fuel will be more accurately simulated under MCCI and ACI engine conditions, which will help guide the identification of fuel property and engine parameter combinations that maximize efficiency and emissions performance.



Major chemical classes with representative components included in the diesel surrogate model. Figure by LLNL

CROSSCUTTING RESEARCH

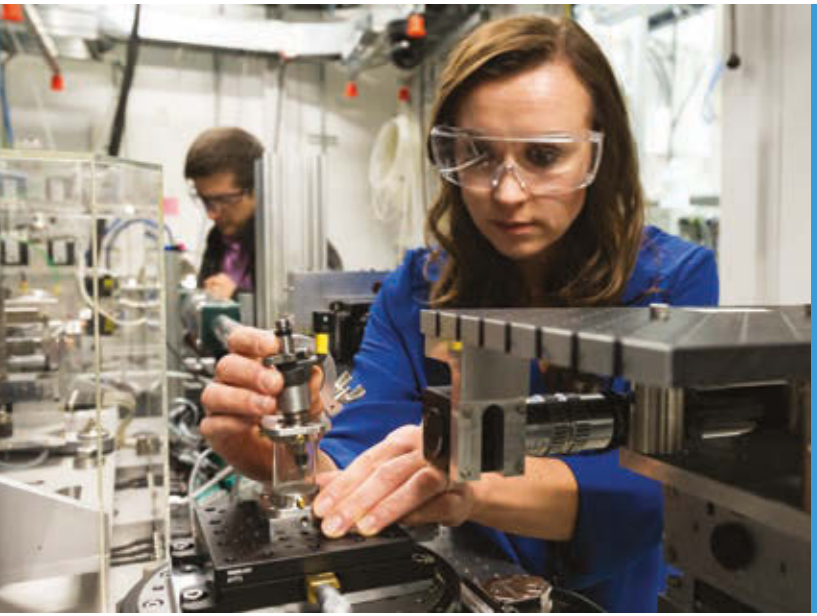
A multidisciplinary approach serves as the foundation of the Co-Optima initiative, and researchers have developed a suite of state-of-the-art experimental facilities and computational tools to advance crosscutting fuel and engine innovations.

Perhaps the most indispensable Co-Optima tool is the boosted spark ignition (SI) merit function. Designed to quantify thermal efficiency benefits in relation to fuel properties, this critical tool has helped researchers better understand fuel-engine interactions, evaluate blendstock candidates, and integrate results from multiple projects within the Co-Optima portfolios.

A broad arsenal of laboratory experimental capabilities supply valuable, highly accurate data on reaction kinetics for fuel ignition and soot formation, which are used in validation of detailed kinetic models and to provide insights into how molecular structure impacts fuel properties. Computational tools utilize and extend this understanding to help identify new blendstocks capable of even greater performance, as well as feasible production routes from biomass.

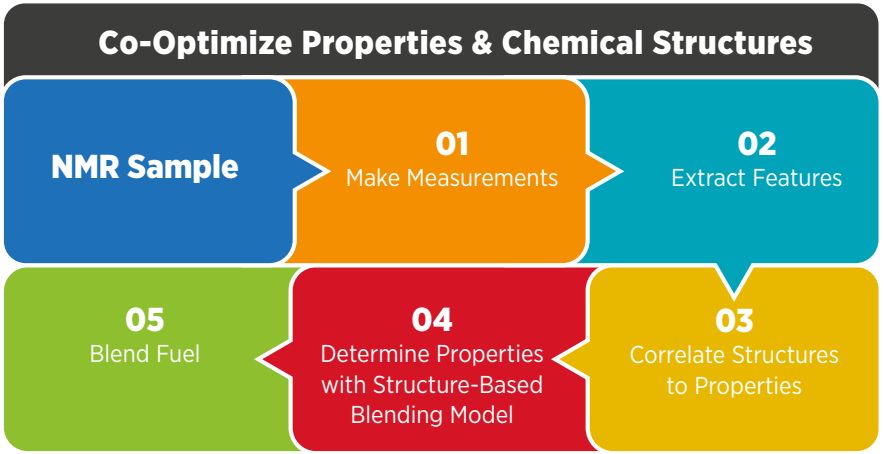
Imaging and characterization tools are being used to increase understanding of how new fuels will change the spray/mixture preparation process, and data on the impact fuel properties have on all engine combustion modes is being captured using high-fidelity predictive simulations. Experiments are also being carried out to understand how new fuel compositions could impact exhaust emission control devices. The development of a new Co-Optimizer software tool makes it possible to assess candidate blendstocks in relation to tradeoffs involving a number of complex variables, including blendstock production scale and economics, life-cycle emissions, and infrastructure compatibility.

The following section highlights activities that benefit from these tools and impact the full spectrum of Co-Optima light-, medium-, and heavy-duty vehicle research.



Fuel Property and Blending Models Built from Chemical Structures in Complex Fuels

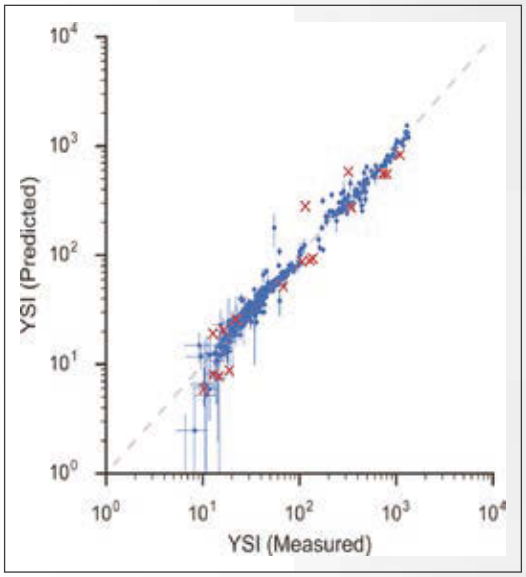
One of the key challenges facing fuels researchers is determining fundamental fuel properties of samples when only very small quantities are available. Co-Optima researchers built statistically-based models relating chemical structures observed in nuclear magnetic resonance (NMR) spectra to key fuel properties—research octane number (RON) or derived cetane number (DCN); simulated distillation values for T10, T50, and T90 (temperatures at which 10%, 50%, and 90% of the volume is recovered during distillation); and Reid vapor pressure. The team built these models using fuel mixtures derived from thermochemical conversion of biomass. Models for each property in the prediction tool are composed of five to seven of the most influential chemical substructures in the complex mixtures. The tool also provides a means of assessing the model fidelity based upon similarity to fuels used for development. By allowing prediction of properties from only 50 – 200 µL of blendstock, which are typically complex multicomponent mixtures, the tool accelerates the rate of early-stage development of new blendstocks. Optimization of fuel blends using chemical structures identified with these models will advance new formulations from both fossil and renewable sources having fuel properties tailored for future engine designs.



NMR spectra of complex fuel mixtures are feature-rich, providing detailed information about the chemical structures within the fuel. Fuel properties, such as distillation (T10, T50, and T90), can be correlated to chemical structures. Multivariate analysis allows optimization of fuel properties from chemical structures as fuel blendstocks are combined to make a target fuel. Figure by Cortland Johnson, PNNL

Sooting Tendencies Predicted for Aromatic and Oxygenated Molecules

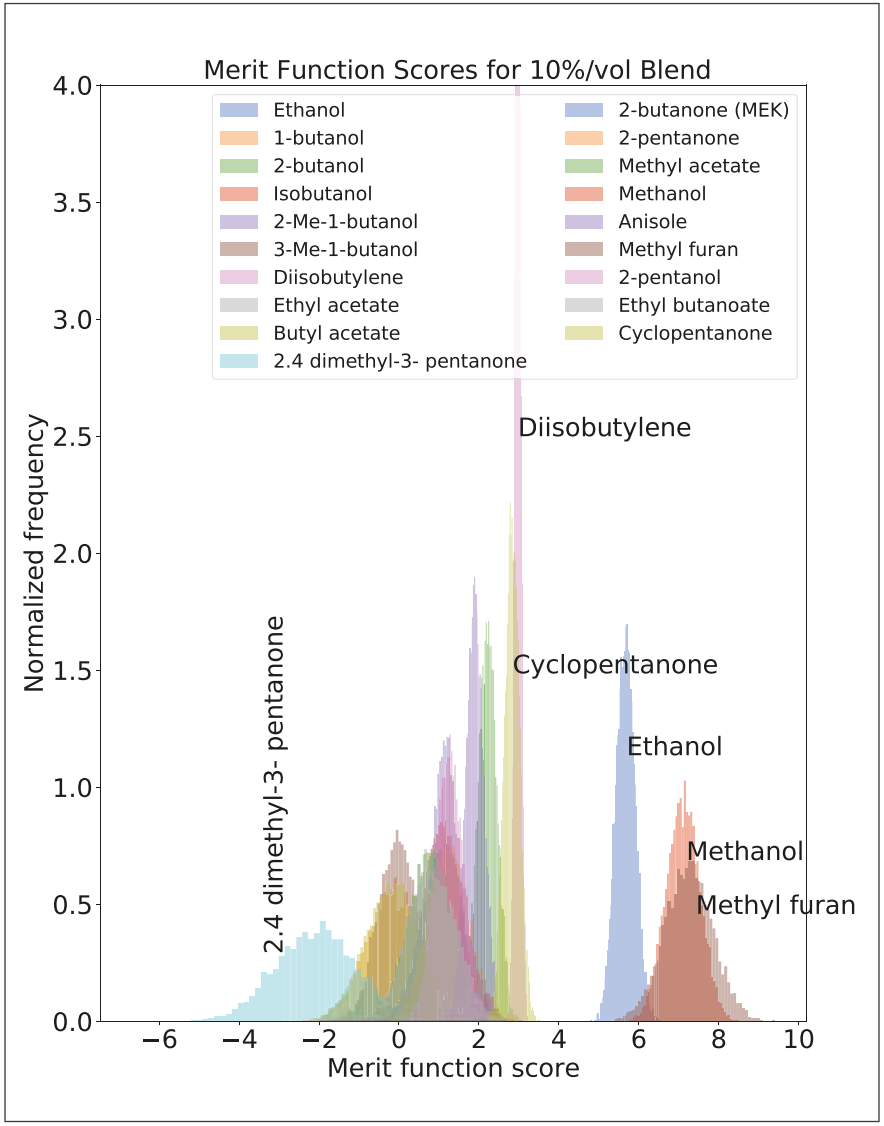
Predicting the sooting tendency of blendstocks is essential for understanding fuel performance in advanced combustion engines, yet is exceedingly difficult because of the very complicated chemical reactions and physical processes that govern soot formation. This includes formation of the first aromatic ring, growth to multi-ring aromatics, particle inception, surface reaction/coagulation, agglomeration, and surface oxidation. Co-Optima researchers developed an improved experimental method with the dynamic range necessary to evaluate the sooting behavior of low-sooting (e.g,. paraffins, oxygenates) and high-sooting (e.g., aromatics) hydrocarbons and a group-contribution model capable of accurately predicting soot formation for a wide range of molecular structures. Outliers of this model typically indicate the presence of more complicated soot formation mechanisms, and these molecules were subsequently further analyzed via density functional theory. This combined approach provides a fundamentally-based, high throughput framework to identify the soot formation tendency of blendstocks directly from molecular structure, helping to guide fuels researchers efforts in assessing the viability of potential blendstocks.



Parity plot of Yield Sooting Index (YSI) model predictions after "leave-one-out" cross validation. Red crosses indicate molecules that are sufficiently different from the remainder of the database for their predictions to be discarded. Figure by Seonah Kim, NREL

Scenario Co-Optimizer Includes Updated Boosted SI Merit Function and Blending Models

Co-Optima researchers are developing the Scenario Co-Optimizer Tool to identify fuel blends that achieve specific fuel quality and performance criteria while meeting user-defined constraints on economic, environmental, and infrastructure compatibility metrics. The Co-Optimizer Tool capabilities were expanded during FY17 to include an interface that allows Co-Optima stakeholders to readily assess the co-optimization potential of a wide array of new fuel options. The Co-Optimizer Tool uses the boosted SI merit function to identify blendstocks that have the requisite properties to maximize engine efficiency when blended into petroleum base fuels. The tool uses Co-Optima-developed blending models to identify fully-blended fuels that meet current fuel quality specifications. User-supplied constraints then identify a smaller subset of solutions that can be compared over a wide range of market introduction scenarios. The current version contains various sample analyses and includes sensitivity analyses to highlight the impact of uncertainty. Results show that changes in the merit function value due to uncertainty in the engine-dependent K factor a constant depending on engine design and operating conditions are small over a range representative of boosted SI operation (-1.25 < K < 0.5), indicating that candidate blendstocks at the 10% level that rank well are clearly distinct from those that do not even when a broad distribution in K is considered. This tool will help guide future R&D and allow stakeholders to identify potential boosted SI fuel options that provide the greatest value propositions for their organizations.



Distribution of merit function values that result from blending candidate blendstocks at the 10% level in a conventional gasoline blendstock for oxygenated blending and drawing 10,000 samples from K distributed as a normal distribution (-1.25; 0.5). Figure by Ray Grout, NREL and Juliane Mueller, LBNL

Reduced-Order Chemical Reaction Model Derived for Fuel Blends

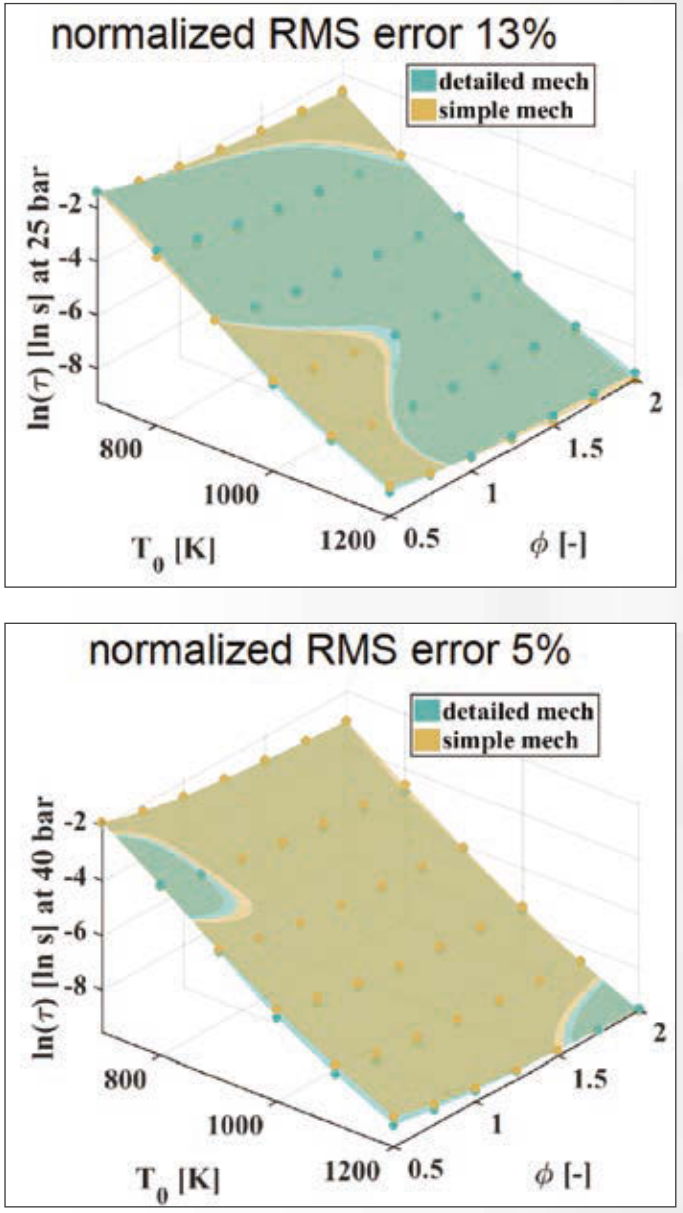
Combustion simulations that include detailed kinetics and turbulence are essential tools for helping to identify optimal combinations of fuel properties and engine design parameters. However, these simulations are extremely computationally demanding, and novel approaches are required to conduct accurate simulations on practical timescales. Co-Optima researchers have developed a reduced-order chemical reaction model for fuel blends that will be used in high-fidelity large eddy simulations at the engine cylinder scale. A complete chemical reaction model even for a simplified surrogate fuel may include thousands of reactions, requiring a reduction in the number of reactions by three orders of magnitude. By functionalizing the Arrhenius parameters with respect to the ignition delay and by using a novel Bayesian inference approach, Co-Optima researchers developed a skeletal three-step chemical model in the following form:

$$C_mH_n+(\tfrac{m}{2}+\tfrac{m}{2})\ 02 \rightarrow m\mathrm{CO}+\tfrac{n}{2}H_2O$$

$$C_2H_5OH+2\ O_2 \leftrightarrow 2\ CO+3\ H_2O$$

$$CO+1/2\ O_2 \leftrightarrow\ CO_2$$

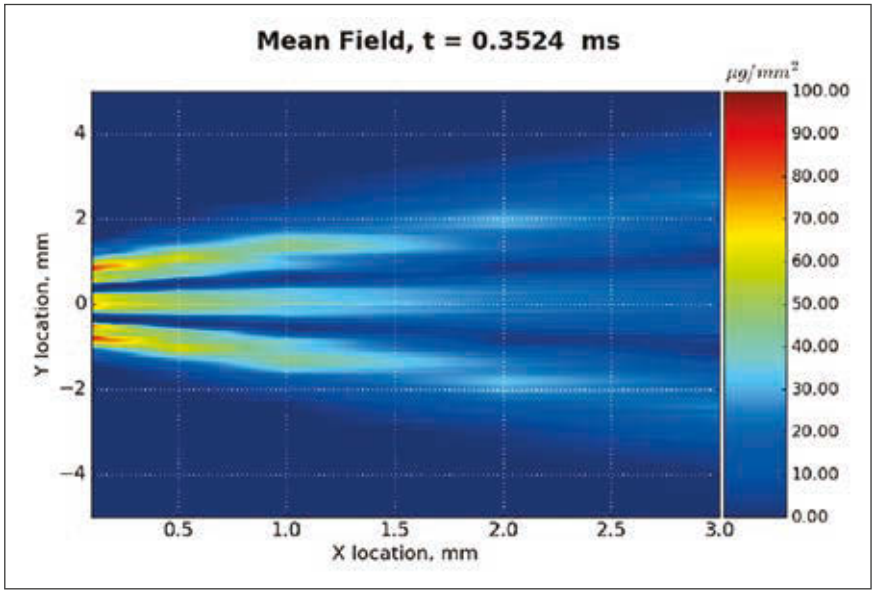
The figure illustrates the method's effectiveness, starting from a detailed reaction mechanism of 5,963 reactions (completely intractable within the large eddy simulation framework) and arriving to a manageable model of only three reactions. At every condition, Bayesian inference finds the most likely surface of ignition delay values. As a by-product, it also generates point-by-point uncertainty bounds which give the modeler a sense of the accuracy of the reduction. This general method is now automated for E10–90 blends. This significant reduction of calculation cost for the chemical reaction term makes accurate large eddy simulations of turbulent combustion practical and affordable, helping to ensure that modeling studies focused on identifying optimal fuel/engine combinations have the greatest possible accuracy.

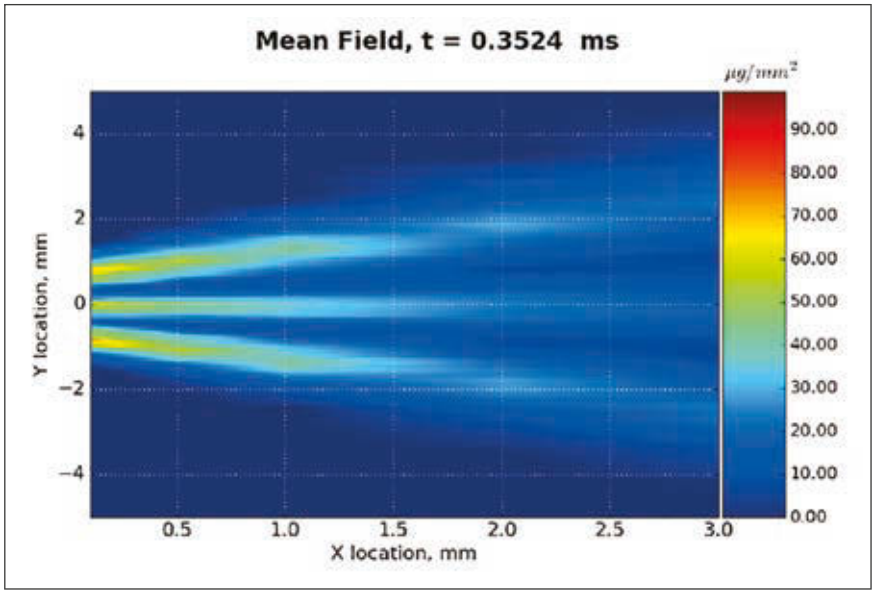


In the two diagrams (mixture pressures of 25 bar, top, and 40 bar, bottom), the logarithm of the ignition delay (in seconds) is plotted as a function of the mixture's temperature (degrees Kelvin) and fuel-air ratio (non-dimensional). Figure by Marco Arienti, SNL

X-rays of Gasoline Direct-Injection Sprays Offer Insights into Fuel Density and Dispersion Effects

Optimizing the performance of direct injection gasoline engines requires a fundamental understanding of the physics governing fuel/air mixing. Co-Optima researchers performed quantitative X-ray measurements of the near-nozzle fuel distribution in gasoline direct-injection sprays to study the effect of fuel physical properties such as density and viscosity on mixture preparation. Researchers compared the time-resolved density distribution of the fuel spray from an eight-hole gasoline direct-injection spray of a gasoline-type calibration fluid with an injection of iso-octane. The iso-octane showed reduced peak density and increased spray dispersion. We believe these are the first ever quantitative measurements of the near-nozzle fuel distribution using flammable fuels. As measurements with additional fuels and fuel blends are completed, the measurements will form a database for the validation of computational simulations of fuel injection, helping to clarify the impact of fuel properties on combustion, efficiency, and emissions.



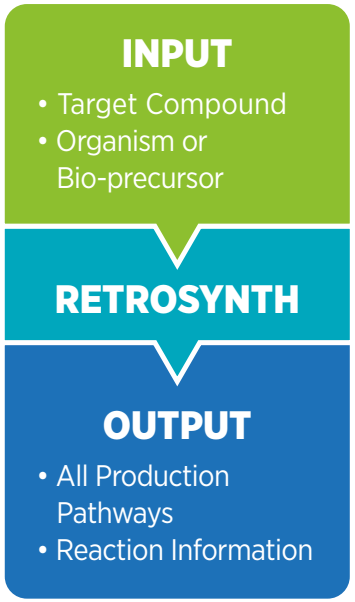


X-rays passing through fuel sprays emerging from an 8-hole gasoline direct-injection injector were projected onto the plane of the detector to reveal the fuel density distributions shown above, color coded in μg/mm². Top is a non-evaporating spray of gasoline-type calibration fluid, bottom is a spray from the same injector using iso-octane. Figure by Christopher Powell, ANL

RetroSynth Tool Helps Identify Reaction Pathways to Boosted SI Blendstocks

Identification of a promising fuel blendstock often poses the challenge of assessing how the blendstock can be produced at scale from a variety of biological or chemical processes. Co-Optima researchers developed the RetroSynth Tool based on retrosynthetic analysis—transforming a target molecule into simpler precursor structures through a sequenced approach that is repeated until simple or commercially available structures are realized. Retrosynthetic analysis was conducted on 37 compounds (encompassing eight chemical classes) identified as potential blendstocks for boosted SI fuels. RetroSynth allows researchers to quickly identify the shortest biological or chemical production pathways to a target fuel for a given microbial organism or bio-derived precursor. For biological routes, it predicts the theoretical maximum yield of the target compound, and for chemical routes, it describes important reaction conditions such as catalyst type, temperature, and pressure. Using this tool and manual curation, Co-Optima researchers identified feasible production pathways for all the target boosted SI blendstocks, and identified several common intermediates for chemical and hybrid approaches, including glycerol, furfural, and levulinic acid.

RetroSynth significantly decreases the time needed to identify the reaction pathways, enzymes, and genes that are required to achieve production of target molecules, making it easier for Co-Optima to identify blendstock candidates that significantly improve engine performance.



RetroSynth allows researchers to quickly identify the shortest biological or chemical production pathways to a target fuel for a given microbial organism or bio-derived precursor. Figure: Loren Stacks, SNL

Evaluation of Barriers for New Oxygenated Blendstocks Informs R&D and Analysis

Understanding the hurdles facing commercial introduction of new blendstocks is critical to informing and maximizing the impact and relevance of Co-Optima R&D and analysis efforts. These challenges extend well beyond issues related to the blendstocks' physical and chemical properties. As a first step in assessing these challenges, Co-Optima researchers identified the steps required to legally sell a new fuel and/or vehicle and summarized these in a report (publication pending). Researchers also evaluated representative oxygenate candidate blendstocks for possible barriers including elastomer compatibility with infrastructure and equipment up to the 30% blend range; presence or absence of a technical specification; and current regulatory hurdles (e.g., limitations to blend levels based on oxygen content); and additional factors such as additive compatibility. Researchers focused on which R&D data could help address these hurdles. The evaluation concluded that backward compatibility with current fuel production, delivery, and vehicle infrastructure is the most important barrier, though others (e.g., development of a technical specification) could increase the time required for market introduction. In addition to guiding Co-Optima research and analysis, these results are particularly helpful to industry in deciding which early-stage research candidates are suitable for advancing through their own development, demonstration, scale-up, and deployment efforts.

NEXT STEPS

All Co-Optima blendstock candidates identified to date face challenges and uncertainties that need to be further quantified. In fiscal year 2018, the research team will complete a systematic examination of the boosted spark ignition (SI) candidate blendstocks in relation to:

- Potential to meet fuel economy targets
- Infrastructure and vehicle material compatibility
- Impacts on emissions control systems
- Scale-up requirements for blendstocks sourced from biomass
- Consumer acceptance and market factors
- Stakeholder value propositions.

Standalone boosted SI research will wind down in fiscal year 2018, as research on multimode SI-advanced combustion ignition strategies for light-duty vehicles increases. Researchers will also continue to expand their work to co-optimize medium- and heavy-duty vehicle fuels and engines , as well as establish critical merit factors for advanced compression ignition fuels.

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ACRONYM LIST & GLOSSARY

Acronyms & Abbreviations

ACI.....advanced compression ignition
ANL.....Argonne National Laboratory
BETO.....Bioenergy Technologies Office (DOE/EERE)
BOB.....blendstock for oxygenate blending
CA.....crank angle
CFPG.....catalytic fast pyrolysis gasoline
Co-Optima.....Co-Optimization of Fuels & Engines
CVCC.....constant volume combustion chamber
DCN.....derived cetane number
DFI.....ducted fuel injection
DI.....direct injection
DOE.....U.S. Department of Energy
DSC.....differential scanning calorimetry
EERE.....Office of Energy Efficiency and Renewable Energy (DOE)
EGR.....exhaust-gas recirculation
FTP.....Federal Test Procedure
GCI.....gasoline compression ignition
GDI.....gasoline direct injection
HDV.....heavy-duty vehicle
HOV.....heat of vaporization
INL.....Idaho National Laboratory
K.....engine-dependent factor in octane index
LANL.....Los Alamos National Laboratory
LBNL.....Lawrence Berkeley National Laboratory
LDV.....light-duty vehicle
LLNL.....Lawrence Livermore National Laboratory
LSPI.....low-speed pre-ignition
LTGC.....low-temperature gasoline combustion
MCCI.....mixing-controlled compression ignition
MDV.....medium-duty vehicle
MON.....motor octane number
NMR.....nuclear magnetic resonance
NREL.....National Renewable Energy Laboratory
OI.....octane index
ORNL.....Oak Ridge National Laboratory
PET.....polyethylene terephthalate
PM.....particulate matter
PNNL.....Pacific Northwest National Laboratory
PPS.....polyphenylene sulfide
PTFE.....polytetrafluoroethylene
PVDF.....polyvinylidenefluoride
R&D.....research and development
RON.....research octane number
S.....octane sensitivity
SI.....spark ignition
SNL.....Sandia National Laboratories
TGA.....thermogravimetric analysis
TRF.....toluene reference fuel
VTO.....Vehicle Technologies Office (DOE/EERE)



Glossary

autoignition ..... Spontaneous ignition of a fuel-air mixture without an ignition source

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

CA50 ..... Crank angle at which 50% of the total heat is released

compression ignition ..... Class of combustion modes where autoignition is achieved through compression heating

core fuels ..... Full boiling range fuels used to compare results across different laboratories and experimental platforms

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

merit function ..... Weighting function that signifies the relative importance of critical fuel properties in engine performance

multimode ..... Engine strategies that use different methods of ignition, combustion, and/or fuel preparation depending on engine needs

mixing-controlled compression ignition ..... Combustion process that is controlled by the rate at which fuel and air are mixed to produce a combustible mixture

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

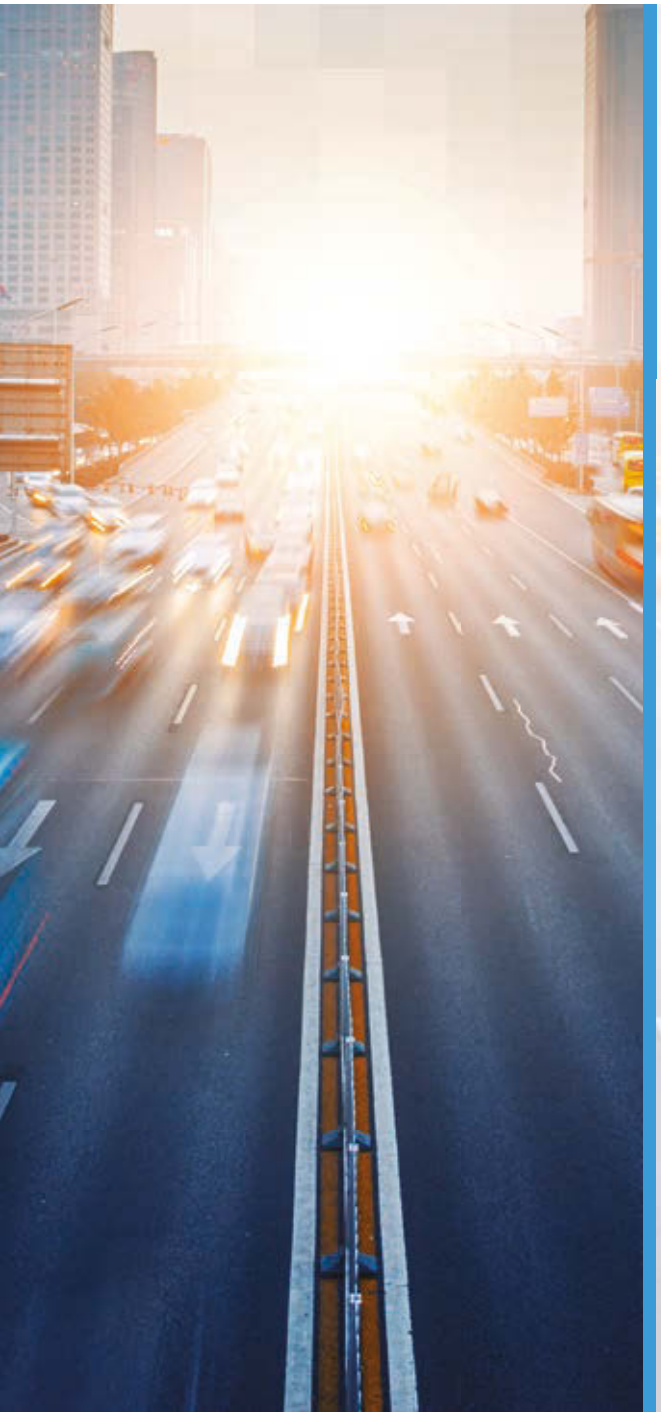
phi sensitivity ..... Extent to which a fuel's autoignition reactivity changes as a function of the fuel-air ratio normalized by the stoichiometric fuel-air ratio

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

sensitivity (S) ..... Difference in octane numbers (RON – MON)

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

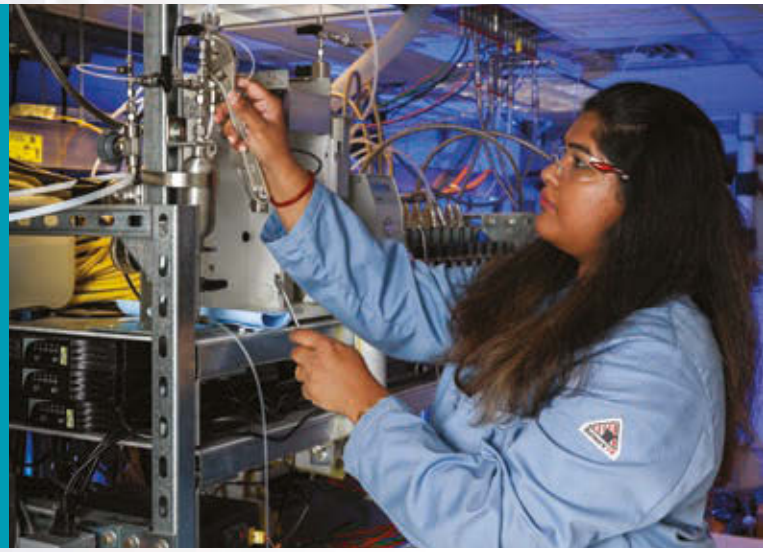
ONGOING DIALOGUE WITH STAKEHOLDERS



Co-Optima leaders continue to engage government and industry decision makers in dialogue to help ensure the success of this initiative. This has taken the form of "listening day" events, participation in trade association meetings, presentations at conferences, visits with individual stakeholders, and input from Co-Optima's external advisory board.

In addition to the two sponsoring EERE offices and national lab partners, Co-Optima has involved representatives from other government agencies at multiple levels, the petroleum and biofuels industries, automakers and original equipment manufacturers, and trade and consumer groups. In fiscal year 2017, 13 universities joined the Co-Optima initiative, providing additional perspectives and complementary world-class research expertise.

These conversations have helped identify R&D needs, potential risks, and mitigation strategies in the areas of engine efficiency and performance, fuel production and distribution, infrastructure compatibility, and retail sales. The national labs and EERE recognize that continued exchanges with these partners are vital to the ongoing success of the Co-Optima initiative.



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