Co-Optima Capstone Webinar Series

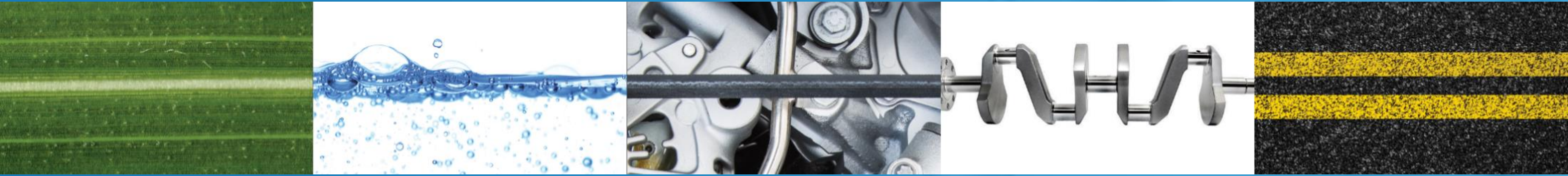
What unconventional engine-fuel combinations show the greatest promise for efficiency improvements beyond current light-, medium-, and heavy-duty technologies?

MAGNUS SJÖBERG – Sandia National Laboratories

Aug 26, 2021

CO-OPTIMIZATION OF FUELS & ENGINES

better fuels | better vehicles | sooner

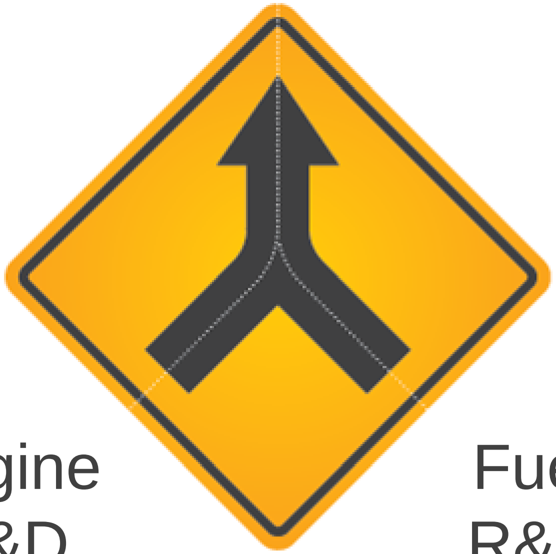


U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

Overview

- Introduction
- Key Take-aways
- Light-Duty (LD) Multimode
- Medium-Duty (MD) / Heavy-Duty (HD) Advanced Compression Ignition (ACI)
- Next Steps

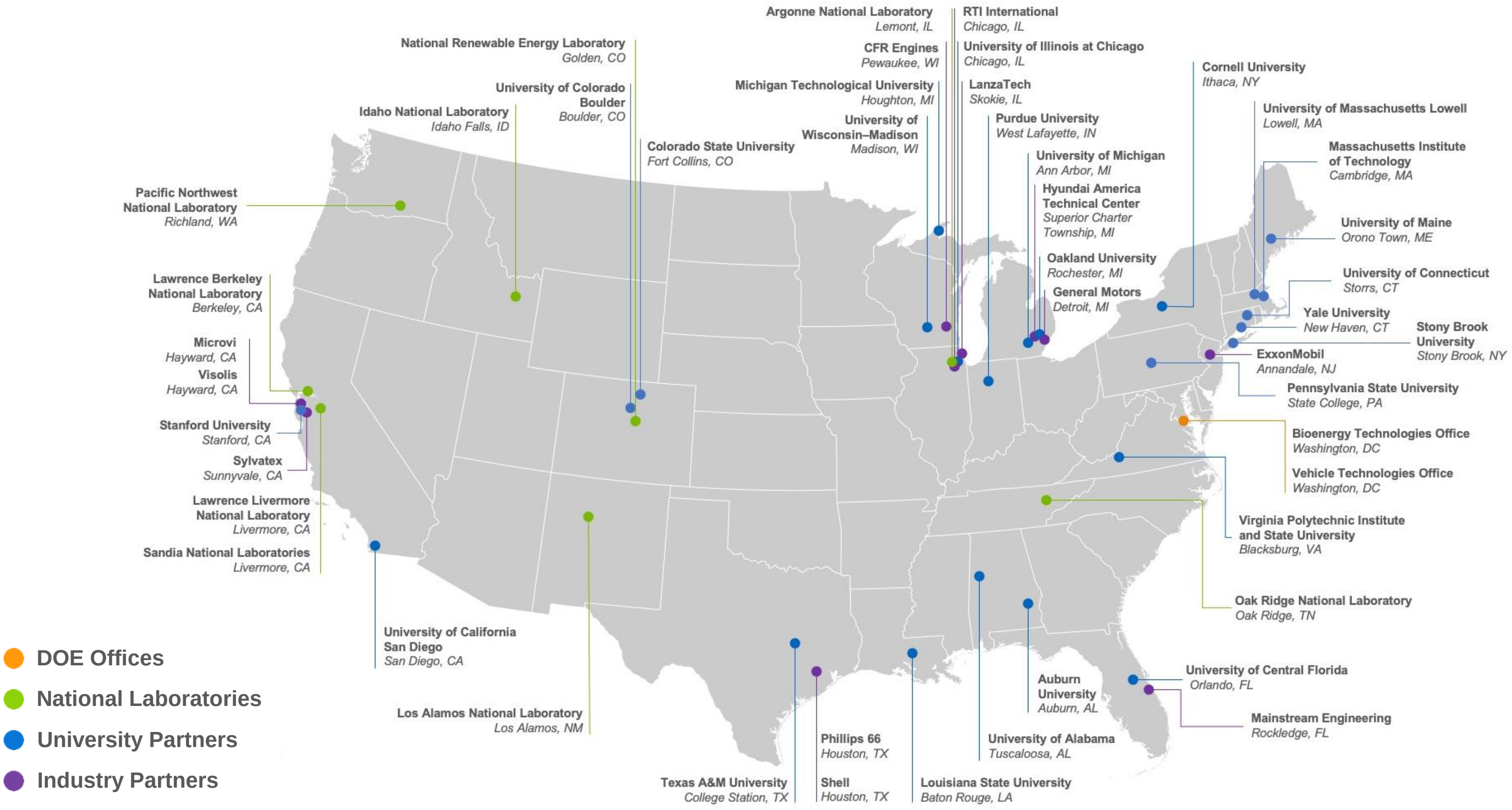
Better fuels. Better engines. Sooner.



Engine R&D

Fuel R&D

Co-Optima draws on national expertise

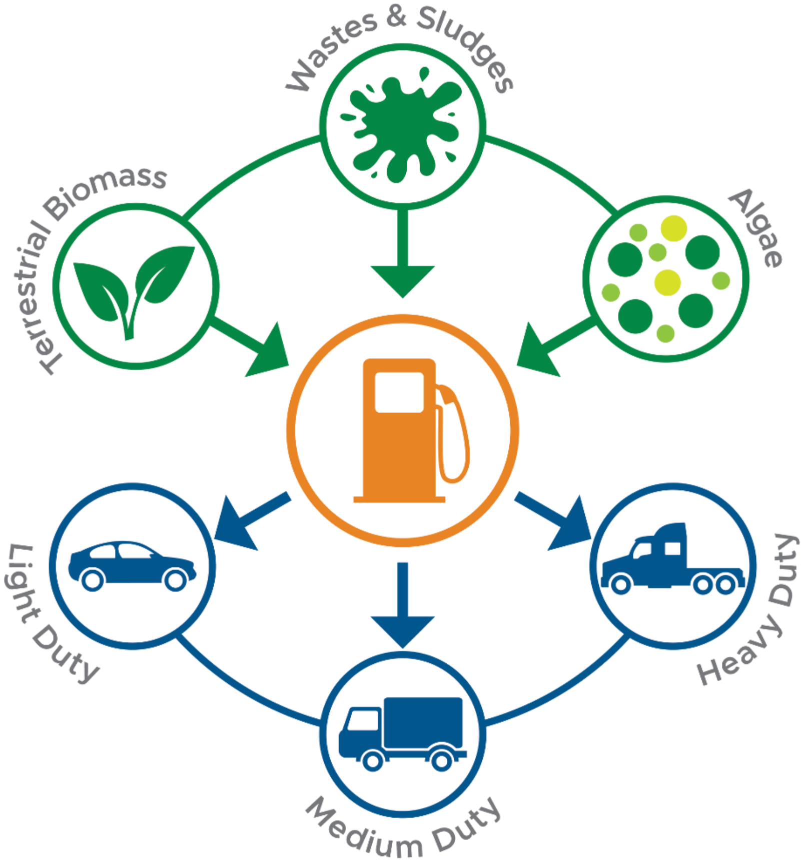


Contributions from across Co-Optima teams

There are many contributors to the work featured in this presentation.

This research was sponsored by the U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE), Bioenergy Technologies and Vehicle Technologies Offices.

Seeking sustainable fuel–engine combinations



- Focus on liquid fuels
- Identify blendstocks
- Consider non-food-based biofuel feedstocks
- Assess well-to-wheels impacts for biofuel options
- Provide data, tools, and knowledge
- Recent focus: up to 30% blend level
- Approach is applicable to high renewable content fuels

Research Approach

Connect engine performance
to fuel properties to fuel chemistry

Link properties to engine efficiency

Hypothesis:

Equivalent fuel properties result in equivalent performance

- Took a fuel-properties-based, composition-agnostic approach
    - However, sometimes new metrics had to be developed (*e.g.*, ϕ-sensitivity)
- Considered new engine designs needed to realize benefits
- Developed new methodologies to quantify how benefits vary with fuel properties

SCOPE On-road transportation from light-duty to heavy-duty

LIGHT-DUTY

- **Near term:** Turbocharged spark-ignition engines
- **Longer term:** Multimode (MM) engine operation

MEDIUM-DUTY / HEAVY-DUTY

- **Near term:** Diesel combustion
- **Longer term:** Advanced compression ignition (ACI)

Today, focus on gasoline-range fuels for both LD & MD/HD

Key Takeaways – MD/HD

ACI with gasoline-range fuels can provide higher efficiency than diesel engines, and with much lower engine-out emissions

Fuels can be designed to provide properties that enable ACI, even at high bioblendstock levels

Key Takeaways – LD

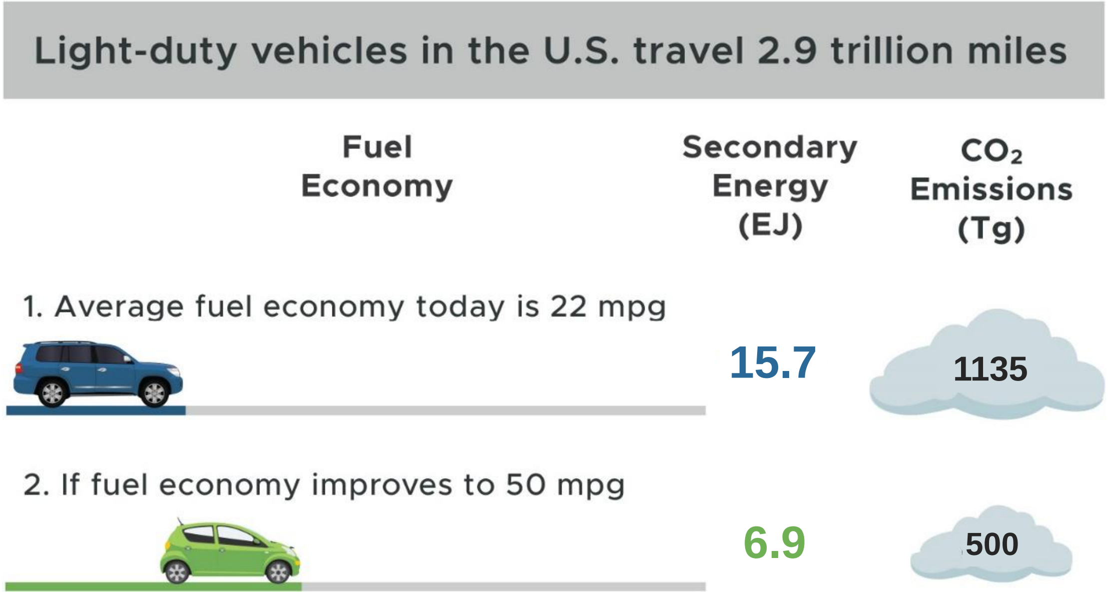
Advanced combustion provides efficiency gains >10% <u>in addition</u> to boosted SI gains

Fuel properties can play an important role to enable advanced combustion

Light-Duty Goal

Determine fuel properties that enable advanced combustion modes with higher efficiency than conventional stoichiometric spark-ignition gasoline engines

GOAL Increase light-duty fleet efficiency



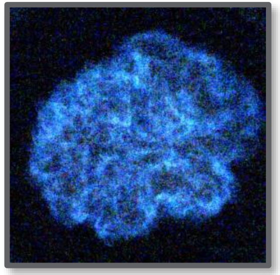
EJ = exajoule Tg = teragram

mpg = miles per gallon

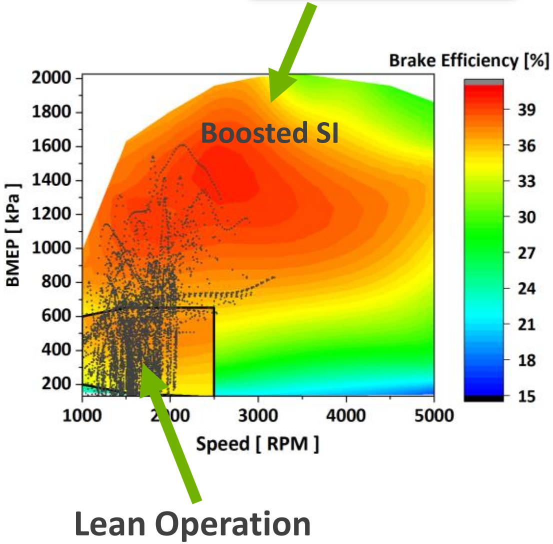
- Increased efficiency lowers fuel consumption and carbon dioxide (CO_2) emissions
- Improved fuel properties can increase engine efficiency
- This applies to both conventional and advanced engine combustion

GOAL Light-duty multimode engine operation

- Multimode uses advanced combustion at lower loads in combination with boosted spark ignition (SI) at high loads
- Goal is to reduce overall fuel consumption
  - What fuel properties enable MM operation?



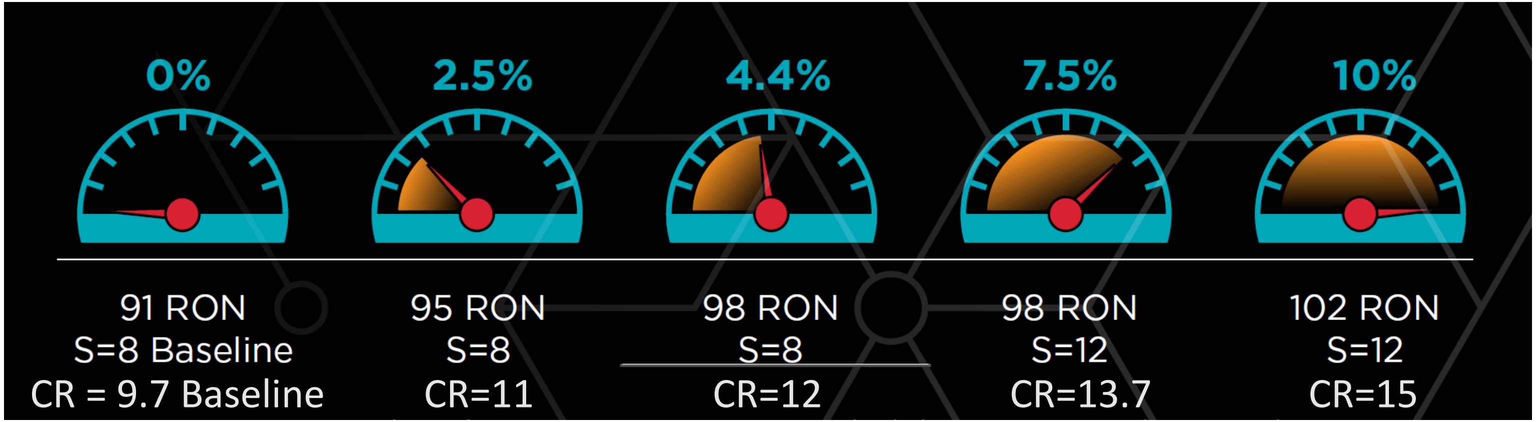
- MM fuels need to enable good low-to-mid load coverage
- MM fuels need to enable boosted SI



Increased RON and S can increase the efficiency of SI engines
(see Co-Optima Capstone Webinar from March 26)

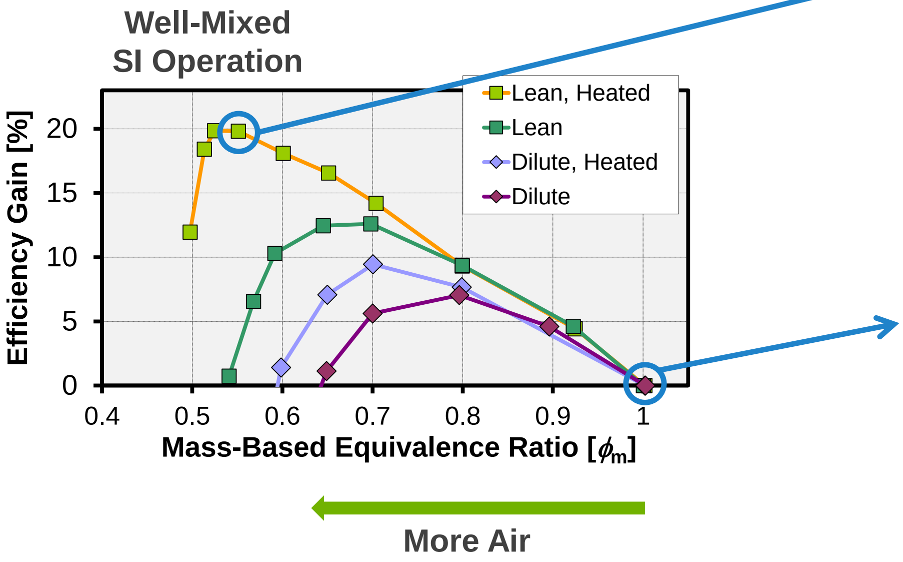
- RON & MON are determined in two different octane tests performed in special test engines
- Octane sensitivity, S = RON - MON

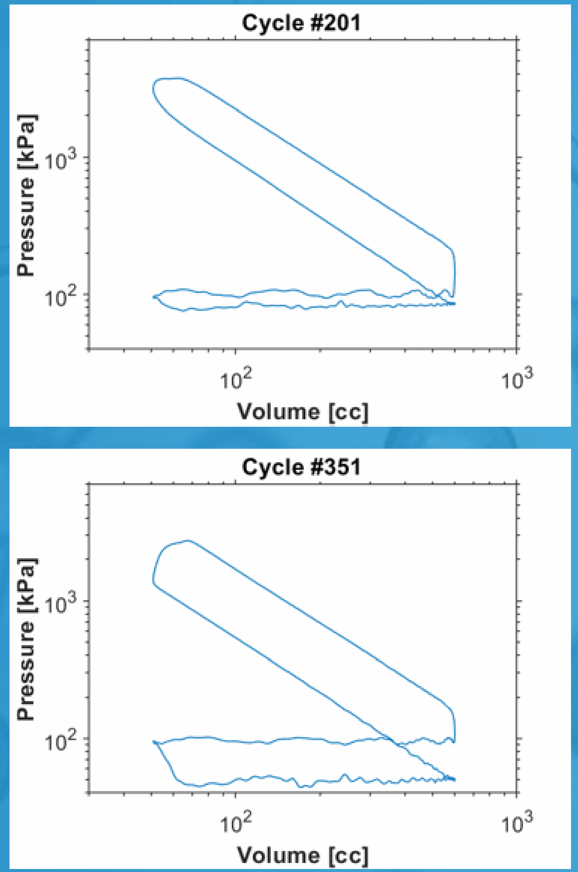
RON = Research Octane Number
MON = Motor Octane Number
CR = Compression Ratio



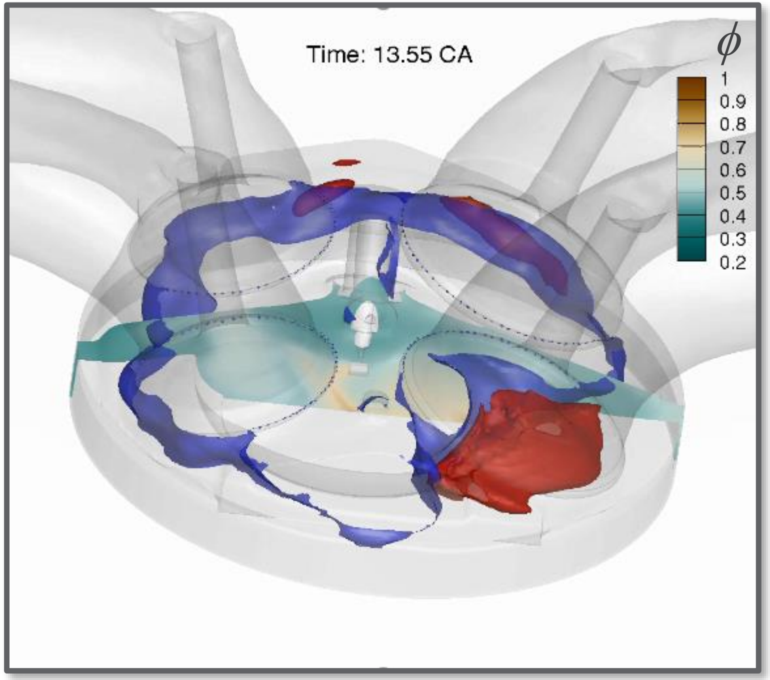
Benefits and challenges with lean operation

- Increased thermal efficiency
  - Improved thermodynamics, reduced pumping losses, and reduced heat transfer losses
- Combustion instability



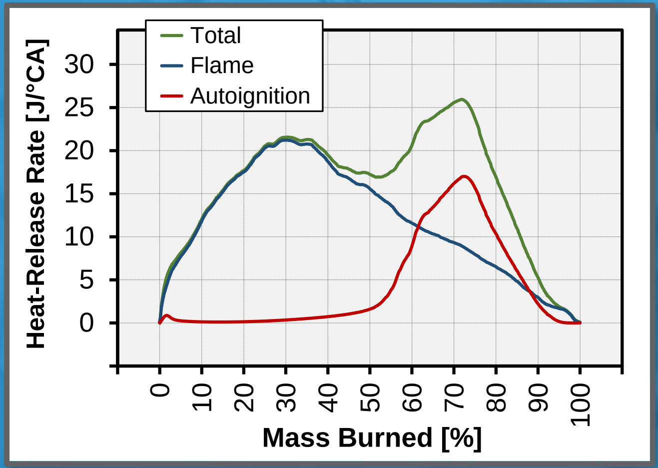


Spark-assisted compression ignition (SACI)



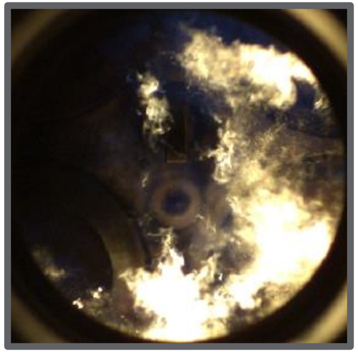
Simulation results of mixed-mode combustion showing how the flame (blue) transitions to end-gas autoignition (red)

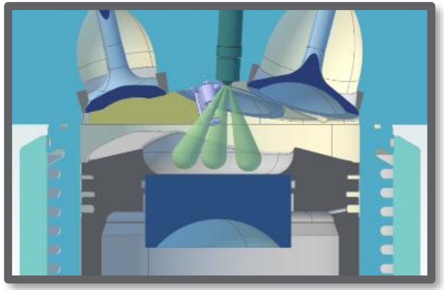
- Partial fuel stratification and spark ignition enable stable lean combustion
- Mixed-mode combustion $\Rightarrow$ sufficiently fast combustion



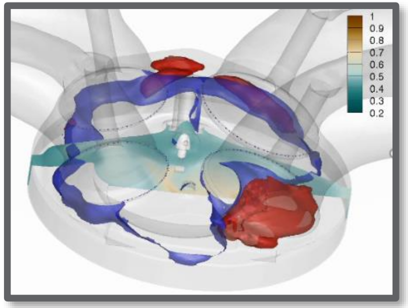
Multiple options for MM engine operation

Stratified Charge (SC)



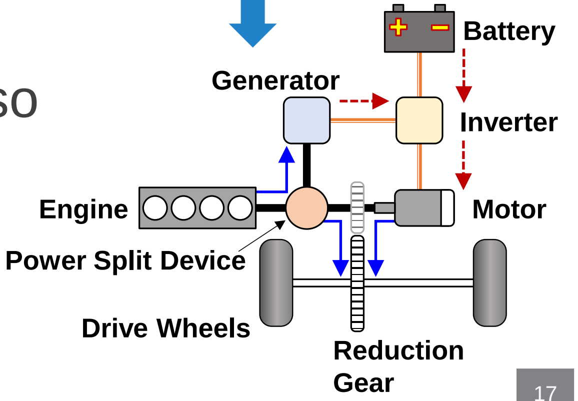


SACI



HCCI

- Examine SACI also for a hybrid powertrain



HCCI = Homogeneous Charge Compression Ignition

What fuel-economy gains are possible?

- Multimode implementation can provide >10% fuel economy gains over boosted SI baseline engine
  - In addition to gains from increased RON & S on boosted SI baseline
  - Multimode in a hybrid powertrain can provide >15% fuel economy gains
- Fuel properties with high impact on SACI load coverage:
  - Higher **RON** = better
  - Higher **S** = better
- Blendstocks with highest potential for improvement:
  - Alcohols (*e.g.*, ethanol)
  - Iso-olefins (*e.g.*, diisobutylene)
  - Alkylfurans

Research Approach

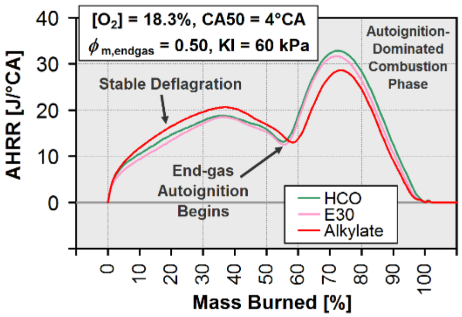
Engine & fuel experiments

Expand combustion parameter space via modeling

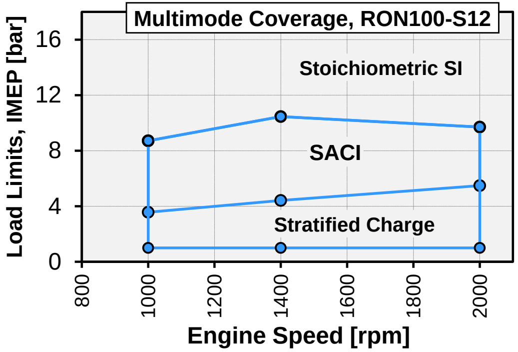
Assess fuel-economy impacts

APPROACH Extend experiments by modeling

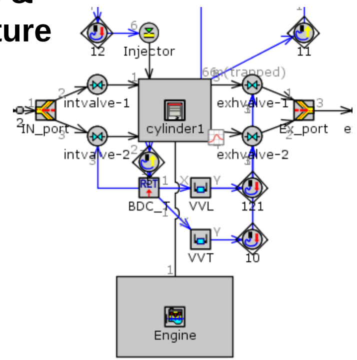
1. Experiments for validation data



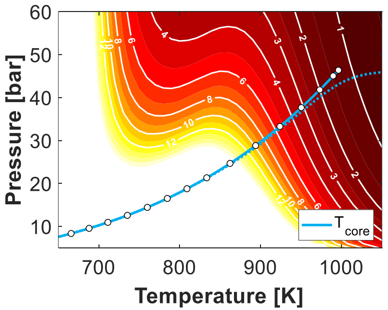
5. Determine fuel economy



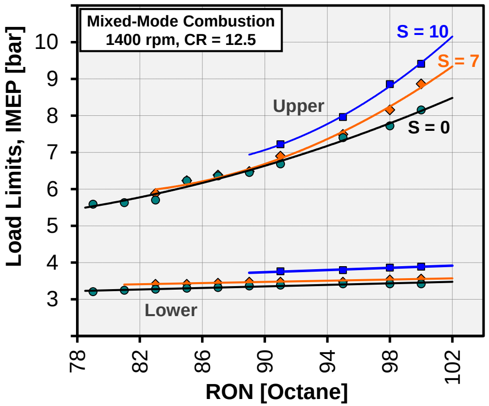
2. GT-Power for pressure & temperature



3. CHEMKIN - Autoignition



4. Quantify load / speed coverage



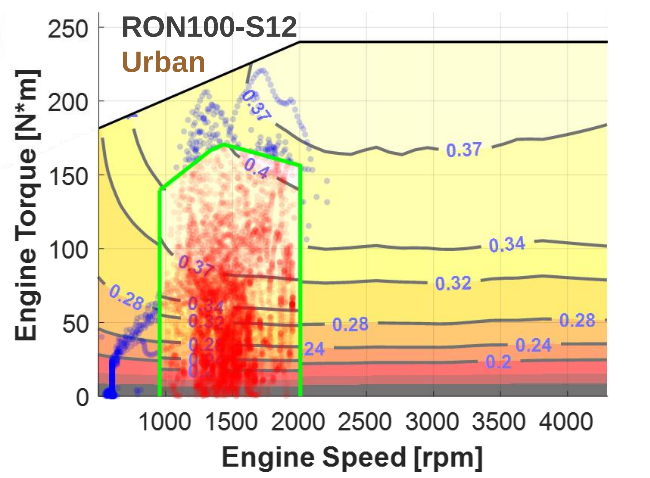
IMEP = Indicated Mean Effective Pressure
rpm = [engine] revolutions per minute

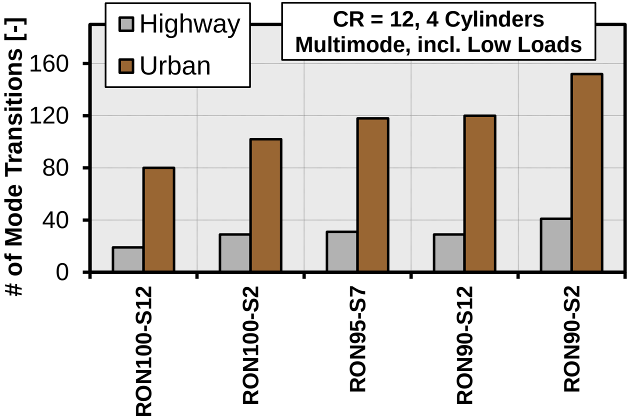
Notable Outcomes

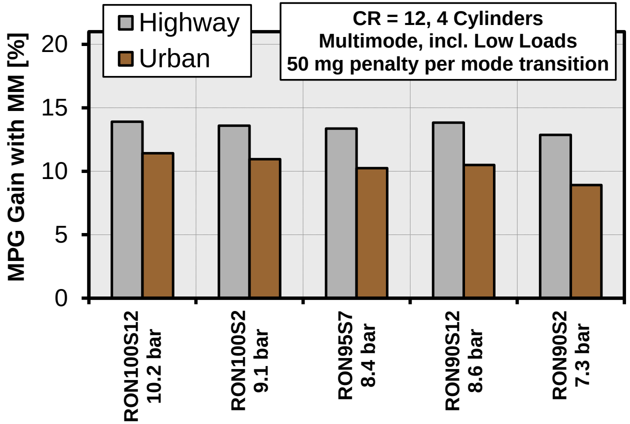
Light-duty fuel–engine co-optimization can achieve >10% fuel-economy gains

OUTCOMES Substantial fuel economy benefits with MM

- Multimode operation provides 9%–14% MPG gains for highway & urban drive cycles
- Mode switching most frequent for urban drive cycle
- Here, the higher SACI load limit of high-RON high-S fuels provides benefits





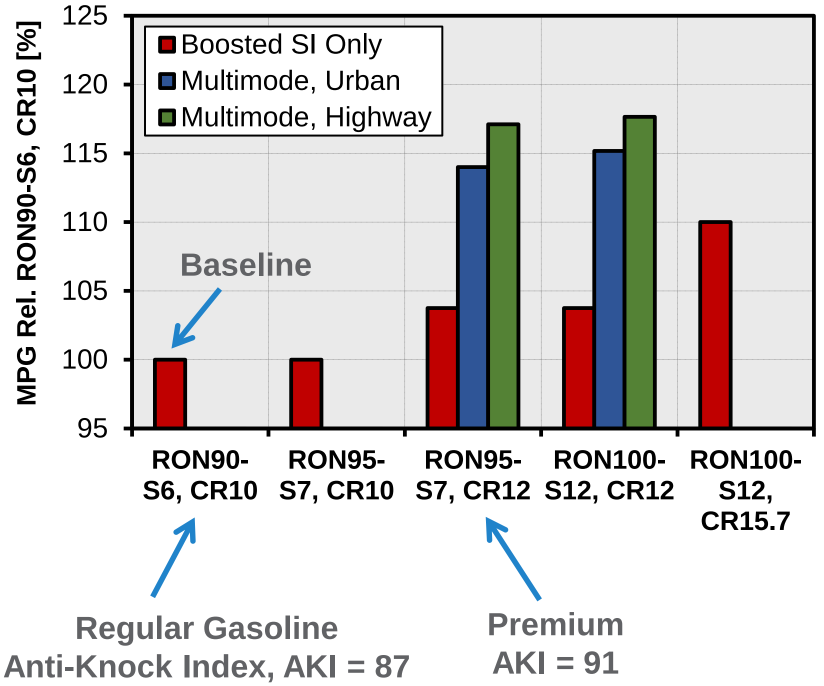


OUTCOMES

Multimode operation provides gains without needing extreme RON & S

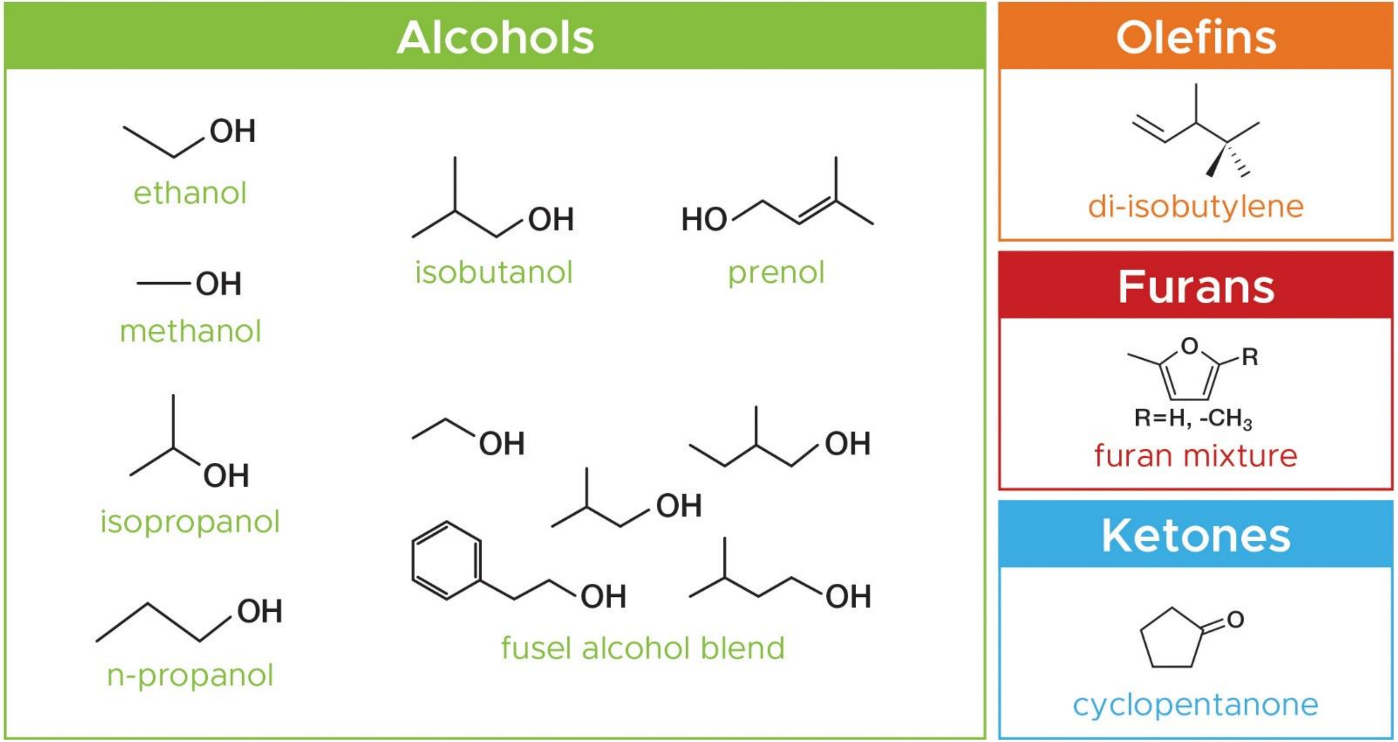
- Here, focus was on CR = 12
- Future work will study effect of CR on multimode operation

- Still, it is clear that:
  – Compared to boosted SI, multimode operation allows substantial fuel-economy gains with less extreme RON & S



Many blendstock options

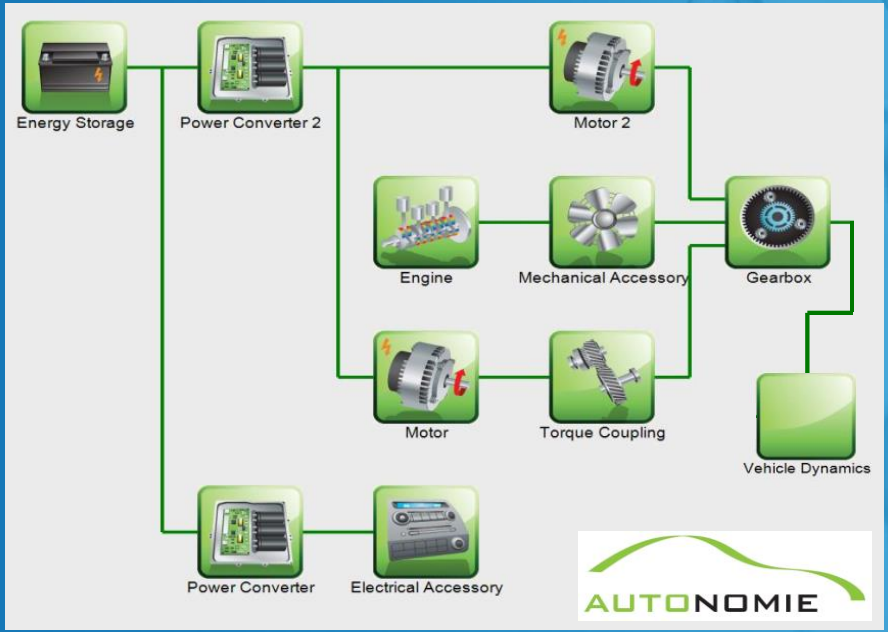
- All have high RON & S
- Smaller alcohols also have high heat of vaporization
- RON for these blendstocks blend synergistically



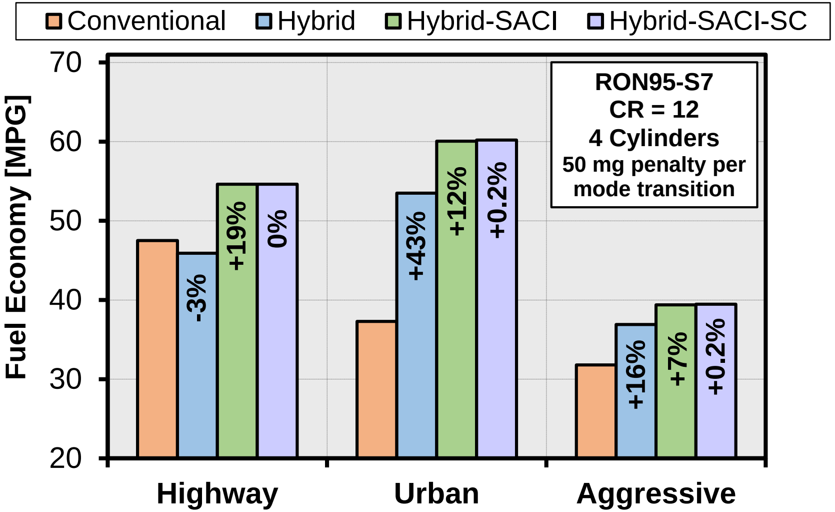
Top 10 Bioblendstocks for Boosted SI Report: https://www.osti.gov/servlets/purl/1567705

OUTCOMES Multimode use in hybrid configuration

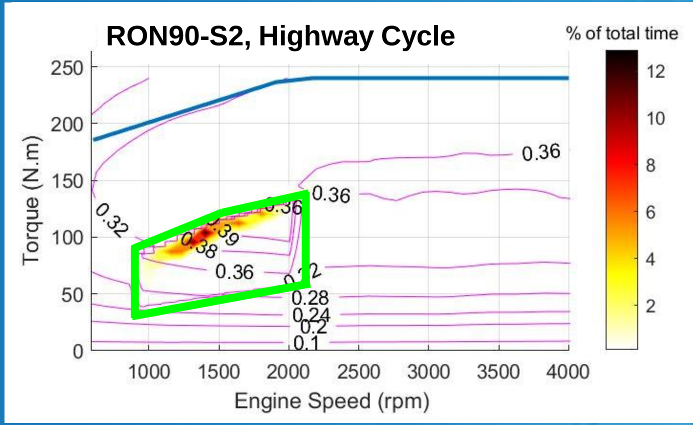
- Power split hybrids create an extremely efficient system
- MPG gains are substantial for both an urban and an aggressive drive cycle (US06)

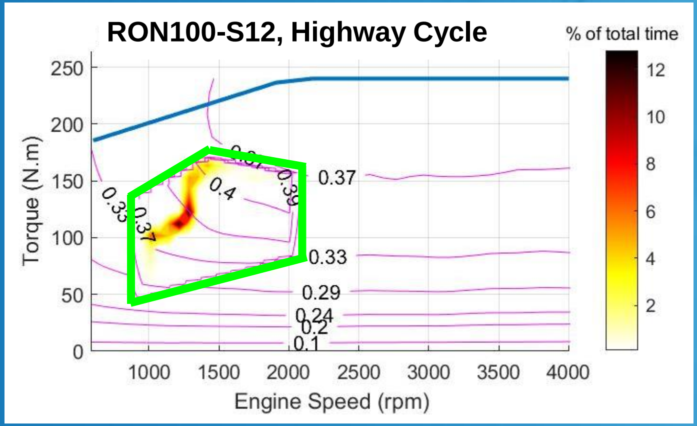


- Multimode engine operation with SACI provides additional gains of 7%–19%
- Stratified-charge SI for lower loads is not required

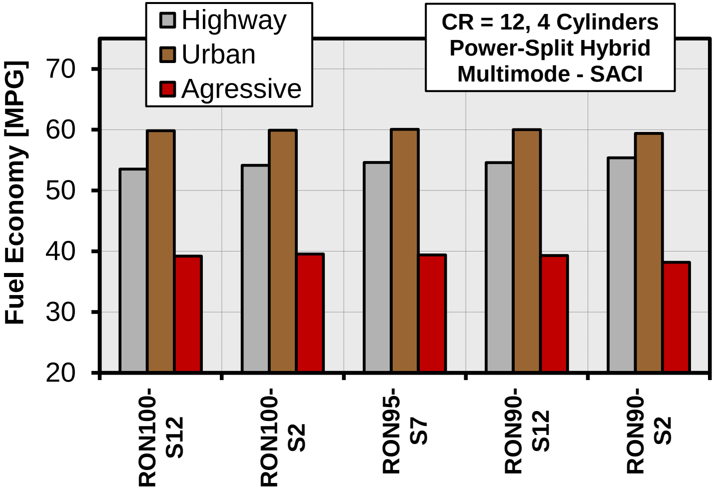


Power-split with SACI - small effect of RON & S





- The HEV adapts to use the most efficient speed–torque areas
- Hence, high fuel economy can be maintained regardless of RON & S



MD/HD Goal

Determine fuel properties that enable implementation of ACI techniques

GOAL Motivation for full-time ACI engine

- ACI engines can lead to high efficiencies and low harmful emissions
  - Ultra-low engine-out NO_x and soot.
- Low-temperature gasoline combustion (LTGC) has demonstrated good performance over the entire operating map
- Efficiencies are 14%–30% above EPA generic 7L diesel

- Bioblendstocks could significantly reduce the carbon footprint of combustion engines
- Can renewable fuels assist LTGC implementation?

NO_x = Nitrogen Oxides
EPA = U.S. Environmental Protection Agency

Research Approach

Engine & fuel experiments

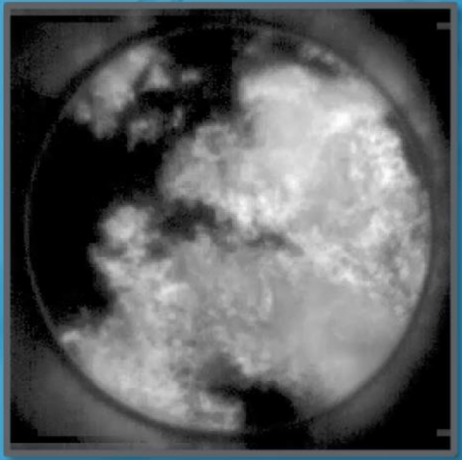
Define new fuel-property metrics

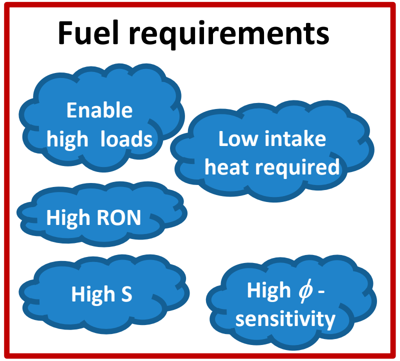
Develop new fuel-blending strategies and expand parameter space via modeling

Extend experiments with modeling

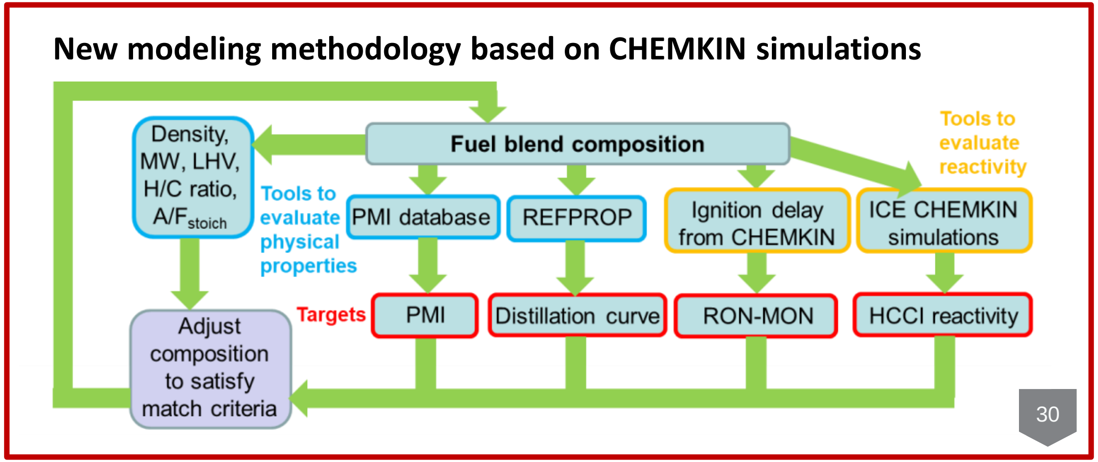
- A new fuel property, ϕ-sensitivity, is important for LTGC operation with partial fuel stratification (PFS).
- Improves combustion control and reduces engine noise

LTGC with PFS





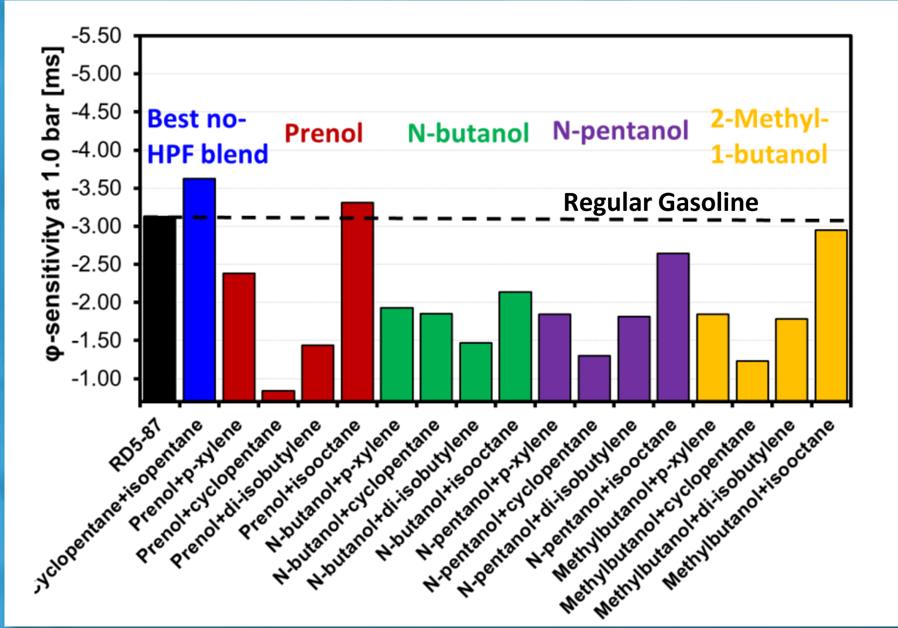
- An LTGC fuel should support ACI operation
- An LTGC fuel should also provide benefits for boosted SI engines



Compare two fuel-blending strategies

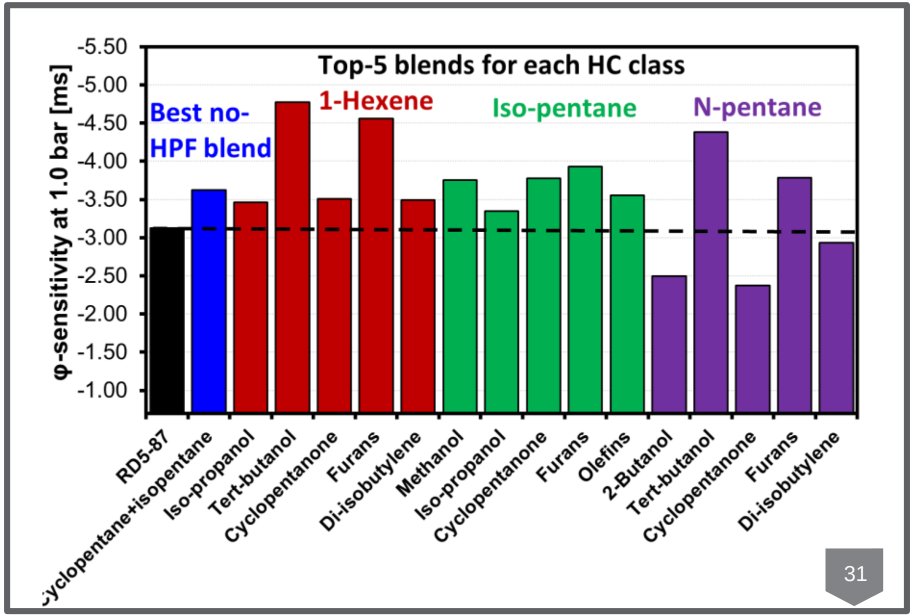
Strategy #1 (not effective)

- High-reactivity bioblendstock provides ϕ-sensitivity + low-reactivity species (provide RON & S)



Strategy #2 (effective)

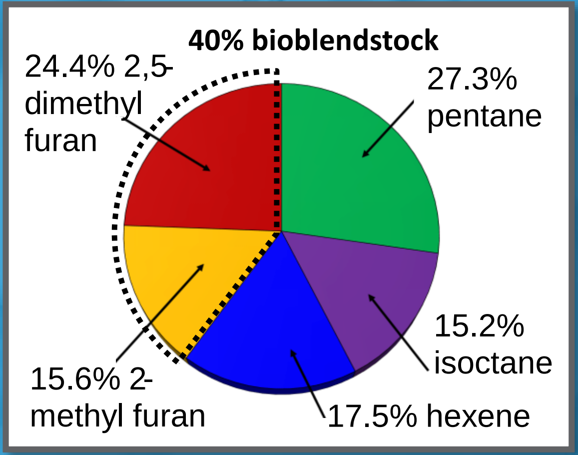
- Low-reactivity bioblendstock provides high RON & S + high-reactivity species (provide ϕ-sensitivity)



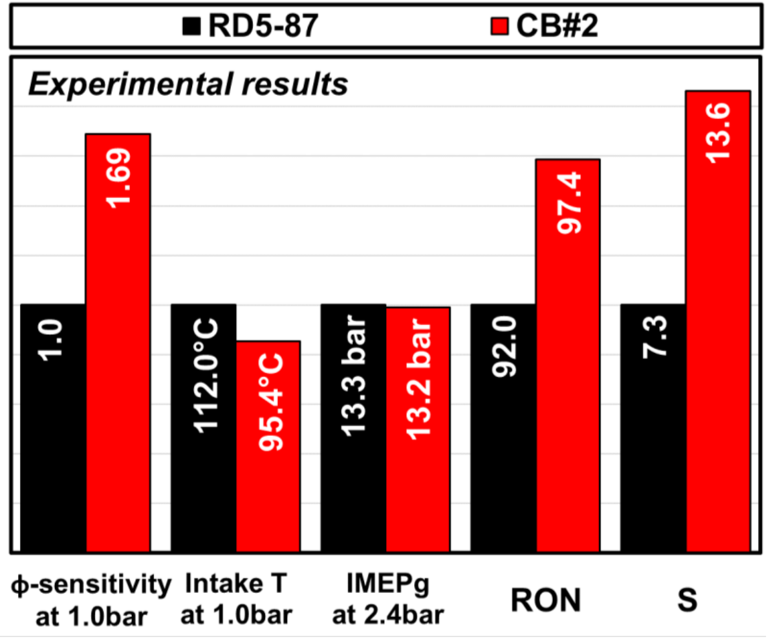
A better LTGC fuel was confirmed experimentally

- A new better fuel, CB#2, was formulated for ACI and boosted SI engines

CB#2 with 40%$_{vol}$ furans.



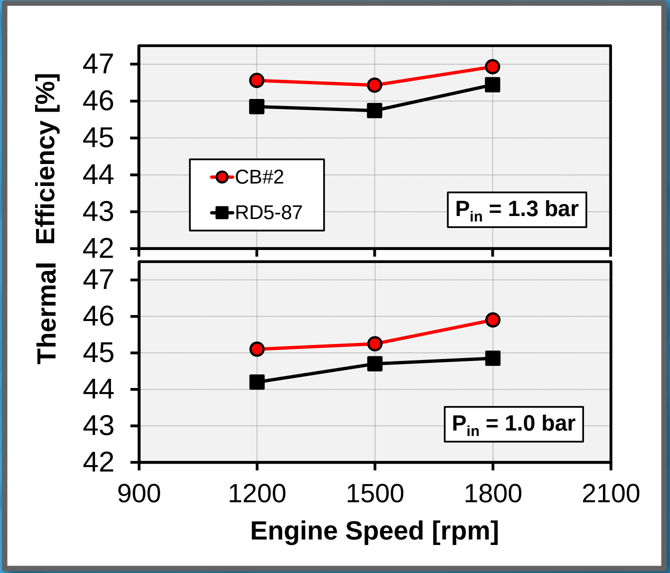
- It has high bioblendstock content and provides higher ϕ-sensitivity, RON, and S



Intake T = Intake Temperature
IMEP$_g$ = Gross Indicated Mean Effective Pressure

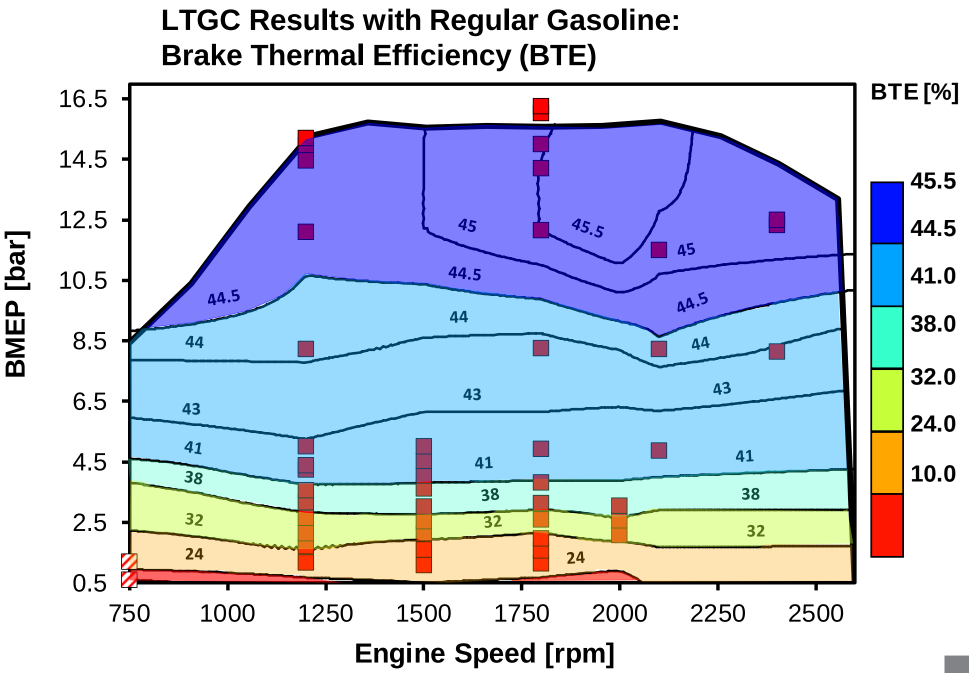
A better ACI fuel provides several benefits

- CB#2 improves combustion control while increasing efficiency



P_{in} = Intake Pressure

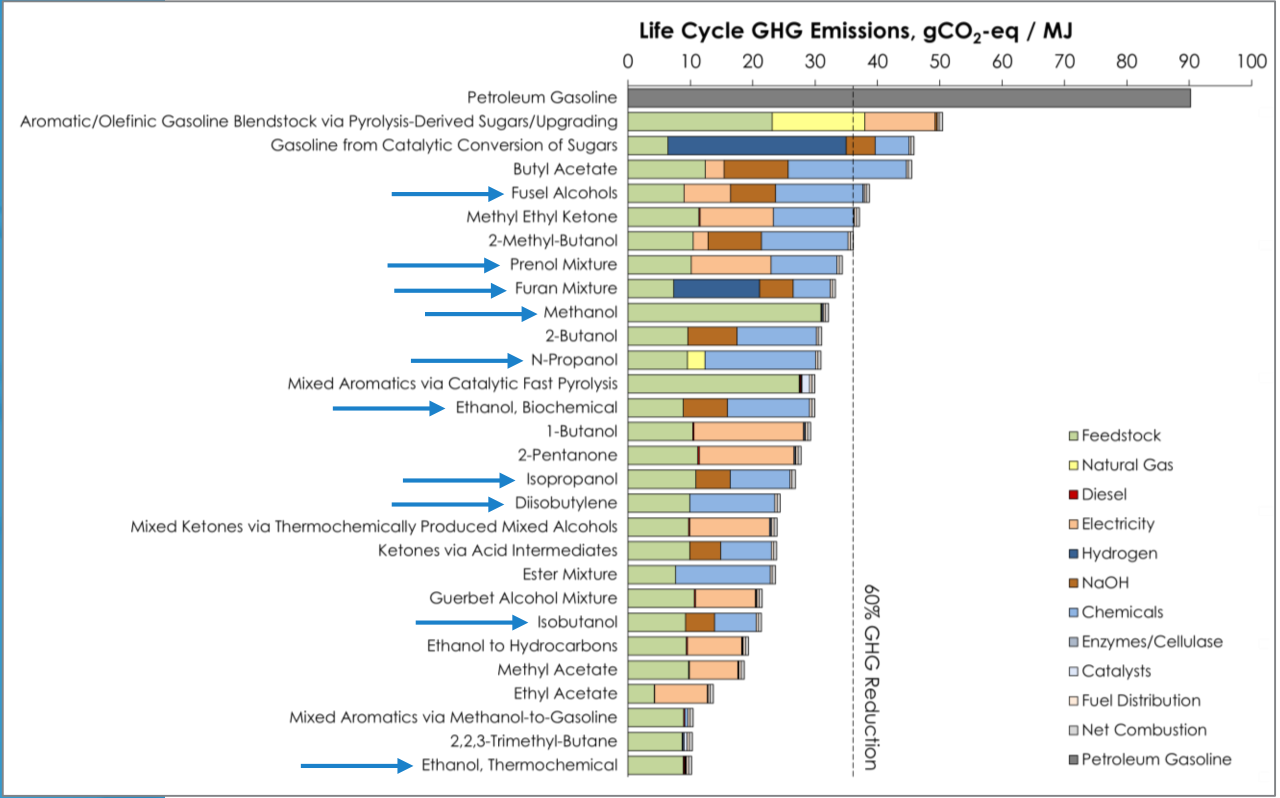
- High bioblendstock content reduces GHG emissions compared to regular gasoline



BMEP = Brake Mean Effective Pressure

OUTCOMES Biofuels reduce GHG emissions

- Wide range of well-to-wheels GHG emissions reductions
- Top candidates all reduce GHG emissions by >50%
- High bioblendstock level + highly efficient ACI engine operation is an attractive combination



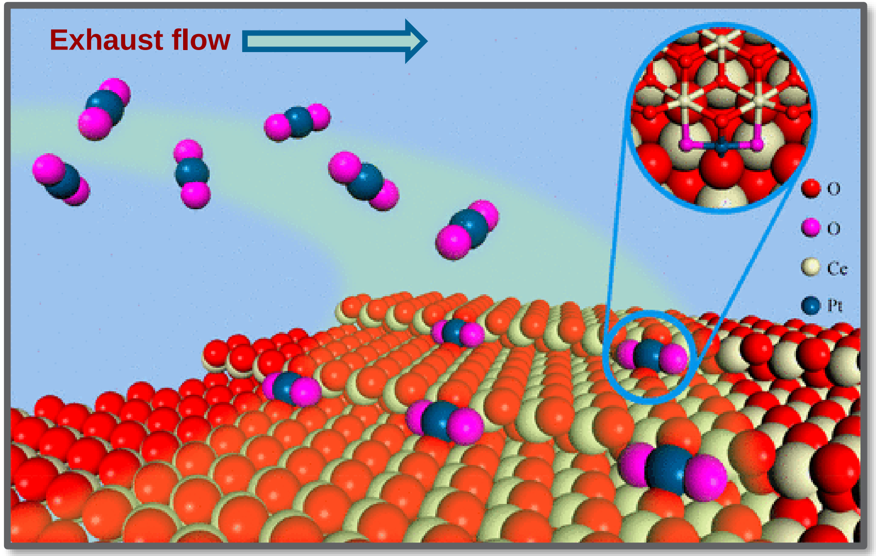
Next Steps

Ensure clean exhaust

Increase blend levels to enable net-zero carbon solutions

Exhaust aftertreatment

- Clean exhaust is imperative for market introduction
- Lean engine operation comes with unique aftertreatment challenges
- Fuel effects have been observed
- Important aspect of fuel-engine co-optimization



Catalyst surface

ACS Catal. 2019, 9, 5, 3978–3990

NEXT STEPS

Realizing the potential

- Scaling up for commercial production
- Overcoming adoption barriers
- Bringing fuels with improved properties - and engines designed to use them - to the marketplace

Energy & Environmental Science

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ANALYSIS

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Cite this: *Energy Environ. Sci.*, 2020, **13**, 2262

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

Jennifer B. Dunn, *[a] Emily Newes,[b] Hao Cai,[a] Yimin Zhang,[b] Aaron Brooker,[b] Longwen Ou,[a] Nicole Mundt,[b] Arpit Bhatt,[b] Steve Peterson[c] and Mary Biddy[b]

Advances in fuel and engine design that improve engine efficiency could lower the total cost of vehicle ownership for consumers, support economic development, and offer environmental benefits. Two fuel properties that can enhance the efficiency of boosted spark ignition engines are research octane number and octane sensitivity. Biomass feedstocks can produce fuel blendstocks with these properties. Correspondingly, using a suite of models, we evaluated the change in energy and water consumption and greenhouse gas and air pollutant emissions in the light duty fleet from 2025 to 2050 when bio-blendstocks isopropanol, a methylfuran mixture, and ethanol are blended at 31%, 14%, and 17%, respectively, with petroleum. These blended fuels increase engine efficiency by 10% when used with a co-optimized engine. In these scenarios, we estimated that petroleum consumption would decrease by between 5–9% in 2050 alone and likely by similar levels in future years as compared to a business as usual case defined by energy information administration projections. Overall, between 2025 and 2050, we determined that, when isopropanol is the bio-blendstock, GHG emissions, water consumption, and $PM_{2.5}$ emission cumulative reductions could range from 4–7%, 3–4%, and 3%, respectively. Cumulative reductions would continue to increase beyond 2025 as the technology would gain an increasing foothold, indicating the importance of allowing time for technology penetration to achieve desired benefits. Annual jobs increased between 0.2 and 1.7 million in the case in which isopropanol was the bio-blendstock. Overall, this analysis provides a framework for evaluating the benefits of deploying co-optimized fuels and engines considering multiple energy, environmental, and economic factors.

Received 6th March 2020,
Accepted 26th May 2020

DOI: 10.1039/d0ee00716a

rsc.li/ees

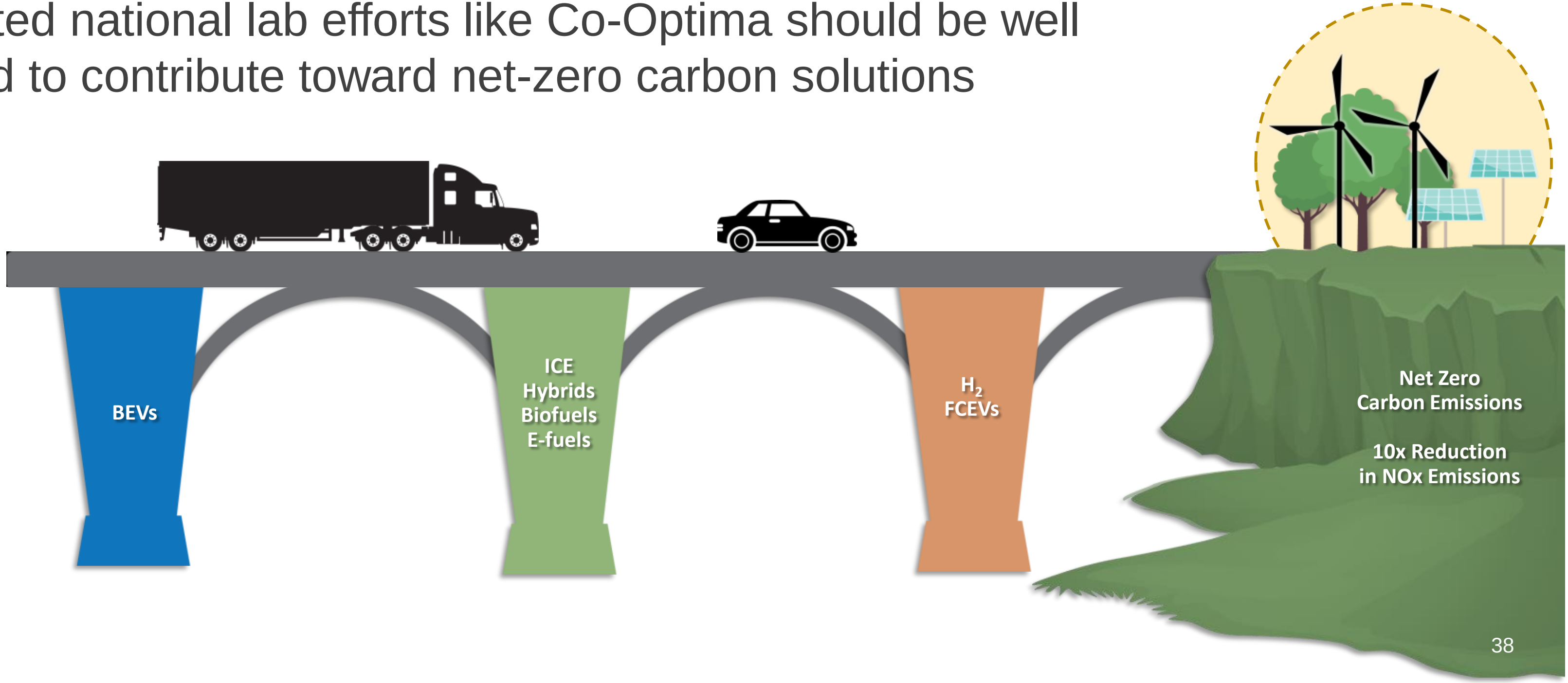
Broader context

Engines and fuels can be co-developed so that engines are designed to exploit unique fuel properties that are exhibited by fuel molecules. In particular, fuel blendstocks derived from biomass have the potential to elevate engine efficiency in boosted spark ignition engines. As vehicles with these engines and the fuels that enable them to achieve higher efficiency enter the market, it is likely that key environmental metrics for the transportation sector, including greenhouse gas emissions, would improve. It is important to consider the influence of this technology deployment on multiple environmental metrics including water consumption and air pollutant emissions and effects on net jobs. In this paper, we use a suite of models to evaluate the energy, economic, and environmental benefits of co-optimized fuels and engines and highlight necessary advances to realize these benefits. Importantly, this analysis goes beyond considering the effects of increasing the renewable content of fuel to consider the additional benefits of engine efficiency gains.

https://doi.org/10.1039/d0ee00716a

Uncertainties in future directions of transportation

- Net-zero carbon emissions pathway may include powertrain technologies that use low carbon and renewable fueled internal combustion engines (ICE), ICE-hybrids, fuel-cell hybrids, and battery-electric powertrains
- Coordinated national lab efforts like Co-Optima should be well positioned to contribute toward net-zero carbon solutions



Acknowledgements Department of Energy

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

Michael Berube
Acting Deputy Assistant Secretary for Transportation

Valerie Reed
Acting Director, Bioenergy Technologies Office (BETO)

Alicia Lindauer
Formerly Technology Manager, BETO Bioenergy Analysis & Sustainability

Jim Spaeth
Program Manager, BETO Bioenergy Systems Development and Integration

David Howell
Acting Director, Vehicle Technologies Office (VTO)

Gurpreet Singh
Program Manager, VTO Advanced Engine and Fuel Technologies

Kevin Stork and Michael Weismiller
Technology Managers, VTO Advanced Engine and Fuel Technologies

Acknowledgements Co-Optima Leadership Team

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Daniel Gaspar
Pacific Northwest National Laboratory

Anthe George
Sandia National Laboratories

Bob McCormick
National Renewable Energy Laboratory

Robert Wagner
Oak Ridge National Laboratory

Capstone webinar series – stay tuned

MAR 25

How can co-optimized fuels and spark-ignition engines enhance efficiency while reducing carbon emissions of light-duty passenger vehicles?

Daniel Gaspar
Pacific Northwest National Laboratory

Jim Szybist
Oak Ridge National Laboratory

APR 29

How can fuels and combustion reduce pollutants from future diesel engines?

Bob McCormick
National Renewable Energy Laboratory

Charles Mueller
Sandia National Laboratories

MAY 27

What environmental and economic benefits might be realized by co-optimizing fuels and spark-ignition engines for light-duty passenger vehicles?

Avantika Singh
National Renewable Energy Laboratory

JUN 24

What environmental and economic benefits might be realized by co-optimizing fuels and engines for medium-duty and heavy-duty commercial vehicles?

Troy Hawkins
Argonne National Laboratory

AUG 26

What unconventional engine-fuel combinations show the greatest promise for efficiency improvements beyond current LD/MD/HD technologies?

Magnus Sjöberg
Sandia National Laboratories

SEP 30

Co-optimization of fuels and engines: past, present, and future—what did we learn and where do we go next?

Robert Wagner
Oak Ridge National Laboratory

Daniel Gaspar
Pacific Northwest National Laboratory

https://www.energy.gov/eere/bioenergy/co-optima-capstone-webinars

Q & A

energy.gov/fuel-engine-co-optimization

energy.gov/eere/bioenergy/co-optima-publications

Magnus Sjöberg
Co-Optima AED Team
Sandia National Laboratories
mgsjobe@sandia.gov