Co-Optima Capstone Webinar Series

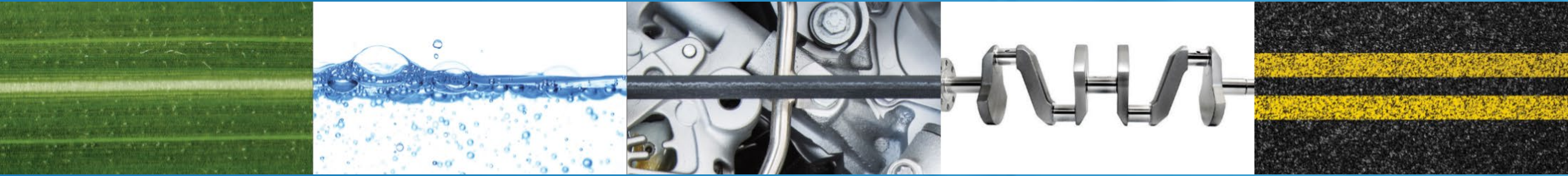
How can co-optimized fuels and engines enhance light-duty vehicle efficiency while reducing carbon emissions?

DAN GASPAR– Pacific Northwest National Laboratory
JIM SZYBIST – Oak Ridge National Laboratory

March 25, 2021

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



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

Overview

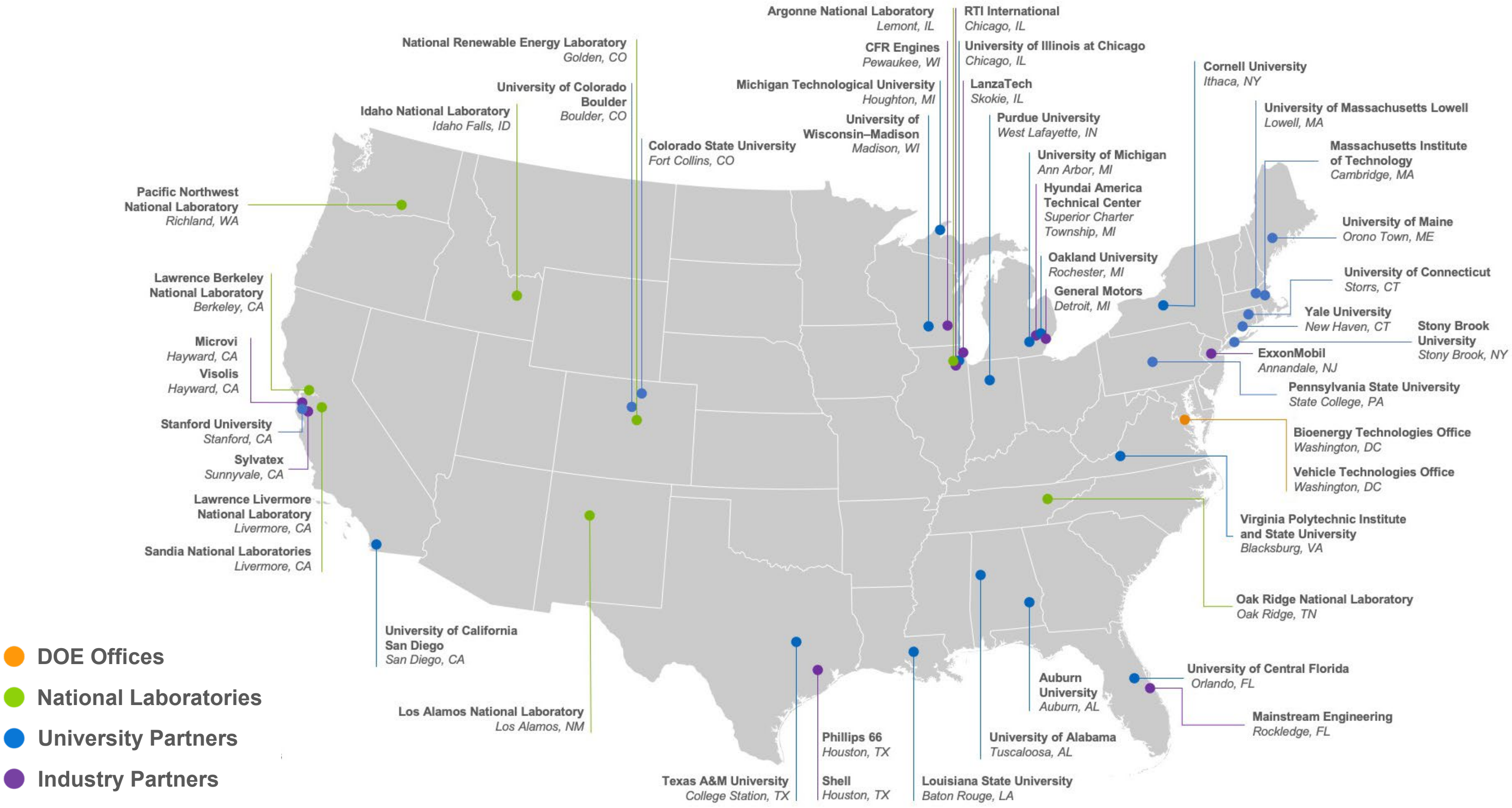
- Goal
- Key Takeaways
- Research Approach
- Notable Outcomes
- Next Steps

Better fuels. Better engines. Sooner.

Engine R&D

Fuel R&D

Co-Optima draws on national expertise



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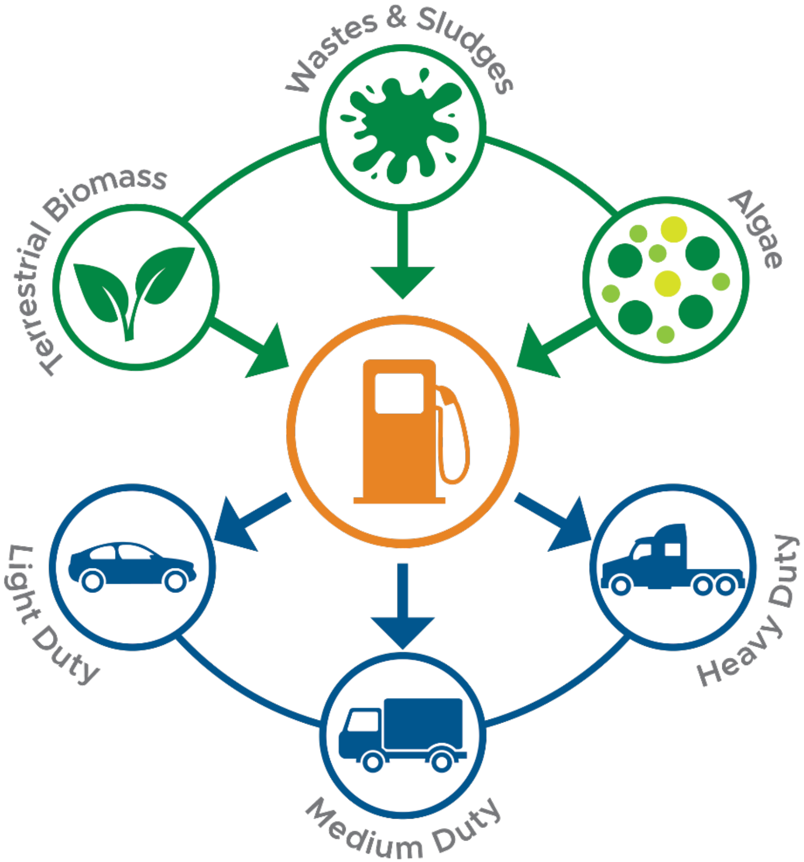
Seeking sustainable fuel-engine combinations



- 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

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

LIGHT-DUTY

- **Near term:** Turbocharged spark-ignition combustion
- **Longer term:** Multi-mode combustion

MEDIUM / HEAVY-DUTY

- **Near term:** Diesel combustion
- **Longer term:** Advanced compression ignition

Capstone webinar series

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?


Troy Hawkins
Argonne National 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?


Avantika Singh
National Renewable Energy 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

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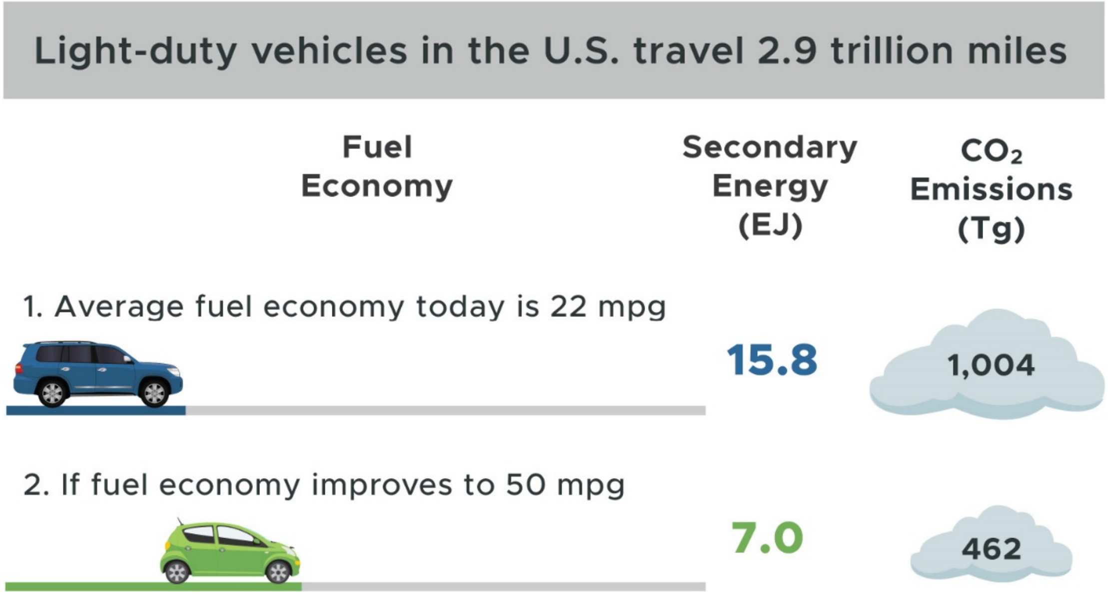
Goal

Identify fuel-engine combinations offering higher efficiency in turbocharged gasoline engines

GOAL Increase light-duty fleet efficiency



Light-duty vehicles in the U.S. travel 2.9 trillion miles

Fuel Economy	Secondary Energy (EJ)	CO_2 Emissions (Tg)
1. Average fuel economy today is 22 mpg	15.8	1,004
2. If fuel economy improves to 50 mpg	7.0	462

Source: 2017, DOT

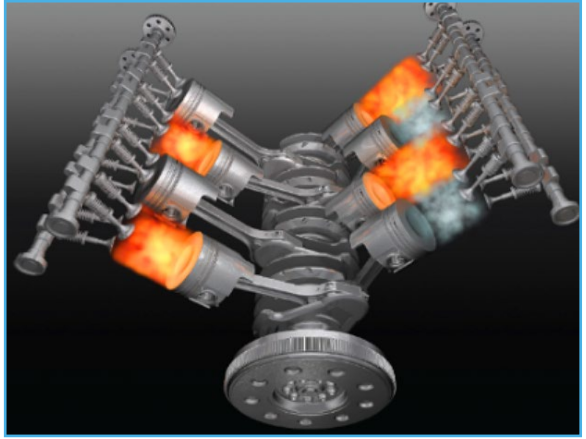
EJ = exajoule

Tg = teragram

- Increased efficiency lowers fuel consumption and carbon emissions
- Improved fuel properties can increase engine efficiency
- Chemical structure-fuel properties-engine performance relationships enable identification of more efficient fuel-engine combinations

GOAL Co-optimize fuels and engines, determine impacts

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

Photos courtesy of iStock

Key Takeaways

Fuel properties enable higher efficiency

TAKEAWAYS What fuel properties are most important?

- Highest impact on efficiency:
  - Research octane number (RON)
  - Octane sensitivity (S)
  - Heat of vaporization (HoV)

- Blendstocks with highest potential for improvement:
  - Alcohols
  - Iso-olefins
  - Alkylfurans

- These can be derived from sustainable sources with reduced life cycle greenhouse gas (GHG) emissions

Research Approach

Connect engine performance
to fuel properties to fuel chemistry

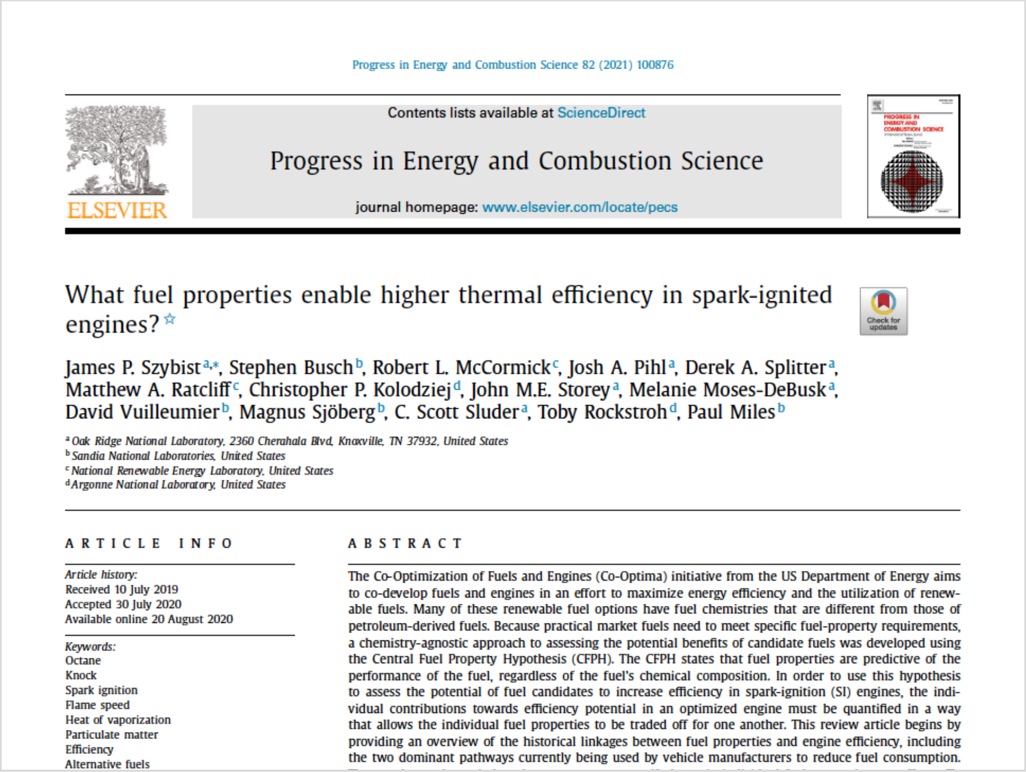
APPROACH Link properties to engine efficiency

Hypothesis:

Equivalent fuel properties result in equivalent performance

- Took a fuel properties-based, composition-agnostic approach
- Considered new engine designs needed to realize benefits
- Developed merit function to quantify benefit potential with properties

Fuel and engine considerations



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

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ABSTRACT

The Co-Optimization of Fuels and Engines (Co-Optima) initiative from the US Department of Energy aims to co-develop fuels and engines in an effort to maximize energy efficiency and the utilization of renewable fuels. Many of these renewable fuel options have fuel chemistries that are different from those of petroleum-derived fuels. Because practical market fuels need to meet specific fuel-property requirements, a chemistry-agnostic approach to assessing the potential benefits of candidate fuels was developed using the Central Fuel Property Hypothesis (CFPH). The CFPH states that fuel properties are predictive of the performance of the fuel, regardless of the fuel's chemical composition. In order to use this hypothesis to assess the potential of fuel candidates to increase efficiency in spark-ignition (SI) engines, the individual contributions towards efficiency potential in an optimized engine must be quantified in a way that allows the individual fuel properties to be traded off for one another. This review article begins by providing an overview of the historical linkages between fuel properties and engine efficiency, including the two dominant pathways currently being used by vehicle manufacturers to reduce fuel consumption.

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Fuel Property Considerations

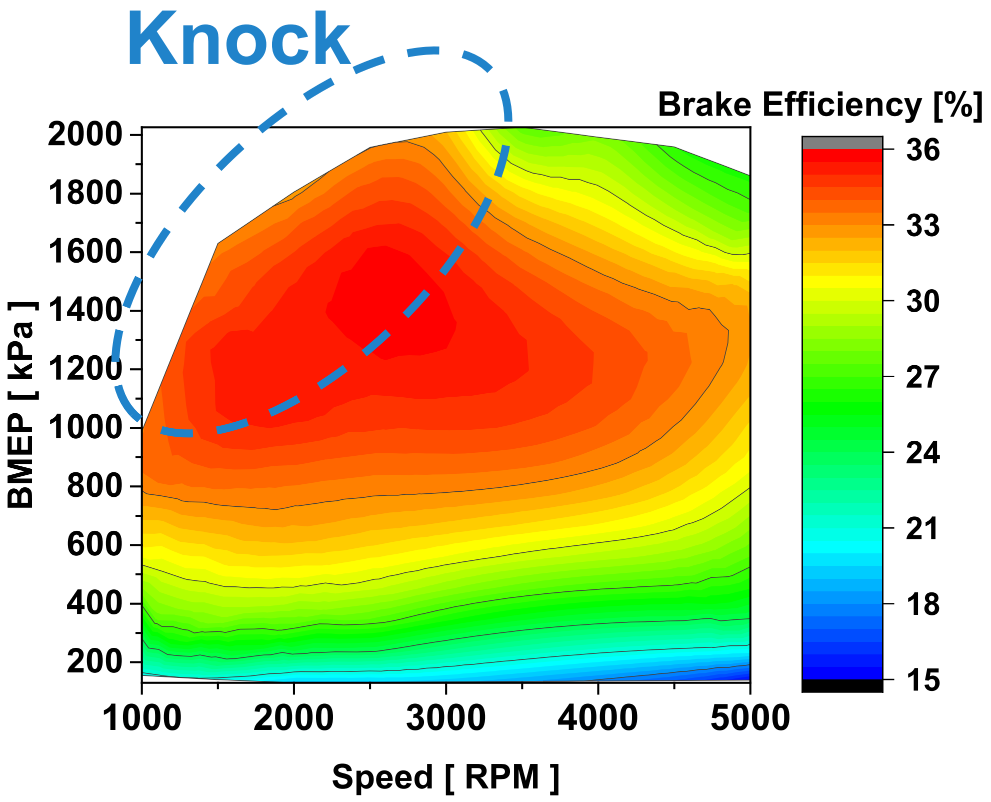
- Fuel candidates screened for >15 qualifying properties
- Detailed analysis conducted on 6 properties for engine optimization

Engine Optimization Considerations

- >6 engine technologies considered for co-optimization

Knock limits engine efficiency

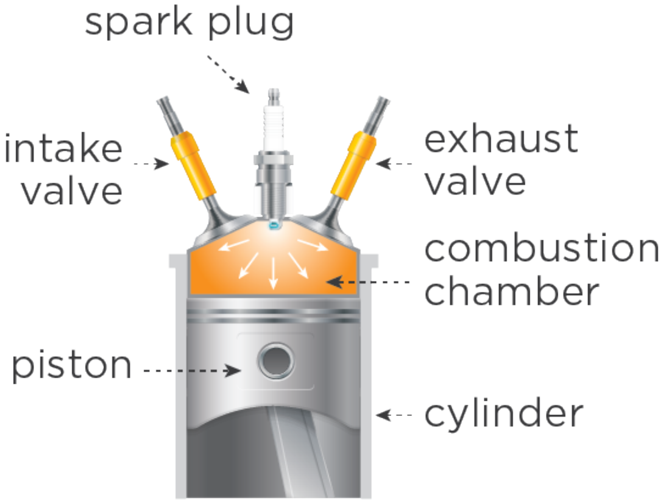
- Engines are most efficient at high load, low speed
- These are also conditions that exacerbate knock and limit efficiency
- Fuels that resist knock can provide higher engine efficiency



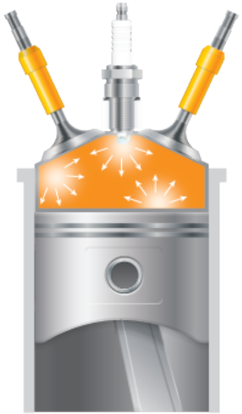
BMEP = brake mean effective pressure, a measure of load

What causes knock?

Knock in unburned gas is promoted by increased *temperature*, *pressure*, and *time*



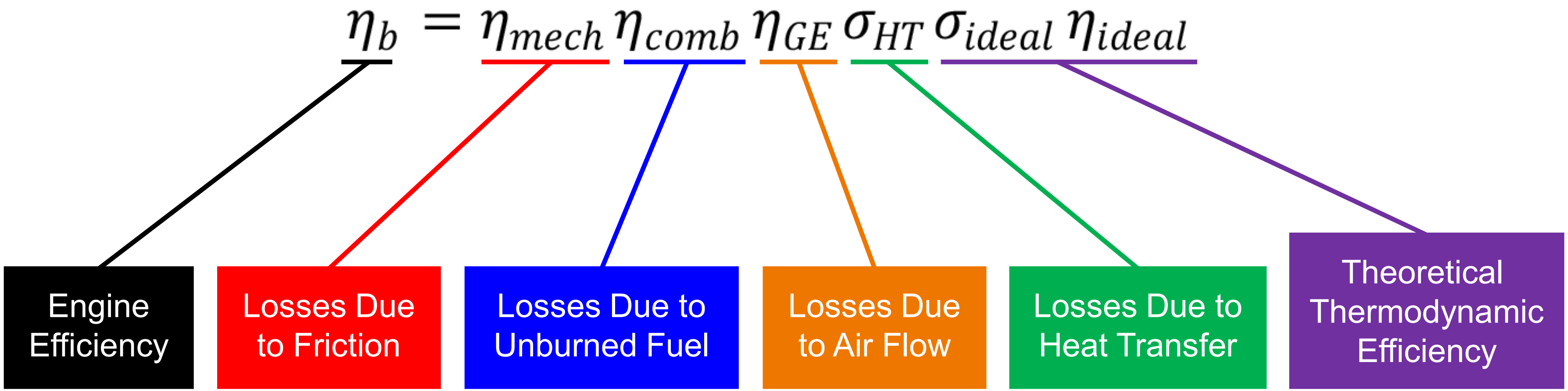
Normal flame propogation
Unburned fuel/air mixture combusts once flame front reaches it



Knock
Unburned fuel/air autoignites before flame reaches it

APPROACH Analyze contributions to efficiency

- Fuel property effects on brake engine efficiency quantified



$$\eta_b = \eta_{mech}\,\eta_{comb}\,\eta_{GE}\,\sigma_{HT}\,\sigma_{ideal}\,\eta_{ideal}$$

Engine Efficiency

Losses Due to Friction

Losses Due to Unburned Fuel

Losses Due to Air Flow

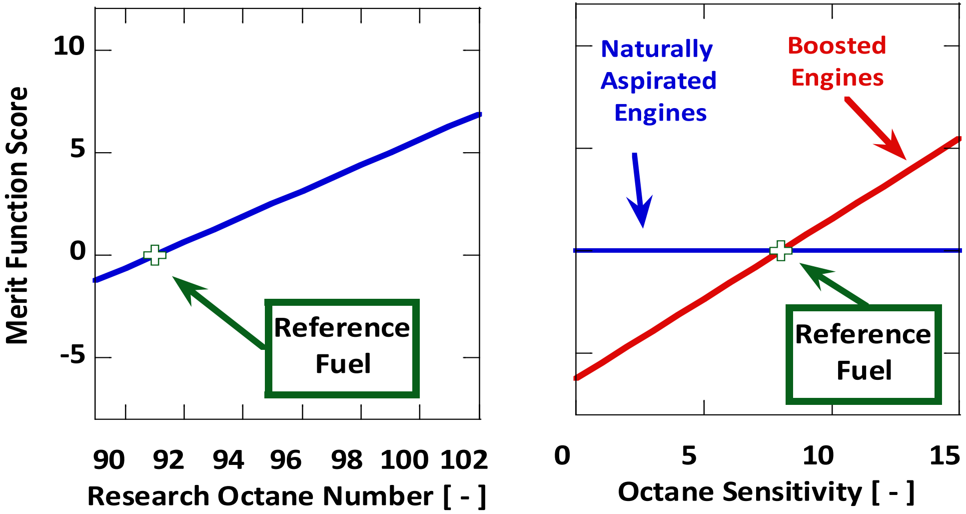
Losses Due to Heat Transfer

Theoretical Thermodynamic Efficiency

- Fuel effects on gaseous and particulate emissions quantified separately

APPROACH Determine efficiency potential of properties

- Considered optimization of engine hardware for changing fuel properties
- Fuel properties that mitigate knock can deliver highest efficiency
    - Research octane number (RON)
    - Octane sensitivity

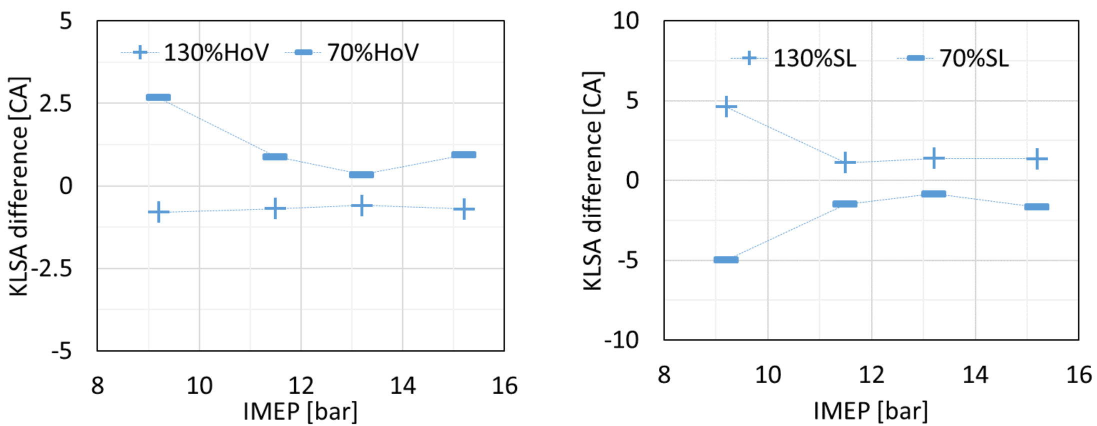


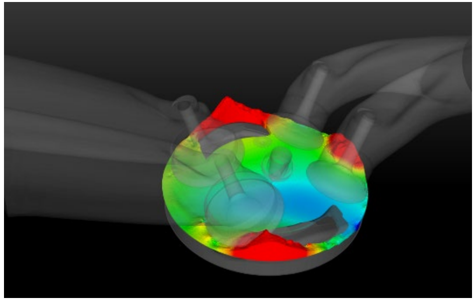
APPROACH Model fuel property effects on knock

- New 3D computational fluid dynamics model can predict knock-limited spark advance (KLSA)
- HOV affects KLSA and knock tendency through its cooling effect in the end-gas region
- *S_L* has significant impact on combustion phasing, which in turn affects end-gas auto-ignition and knock onset

Heat of vaporization (HOV)

Laminar flame speed (S_L)

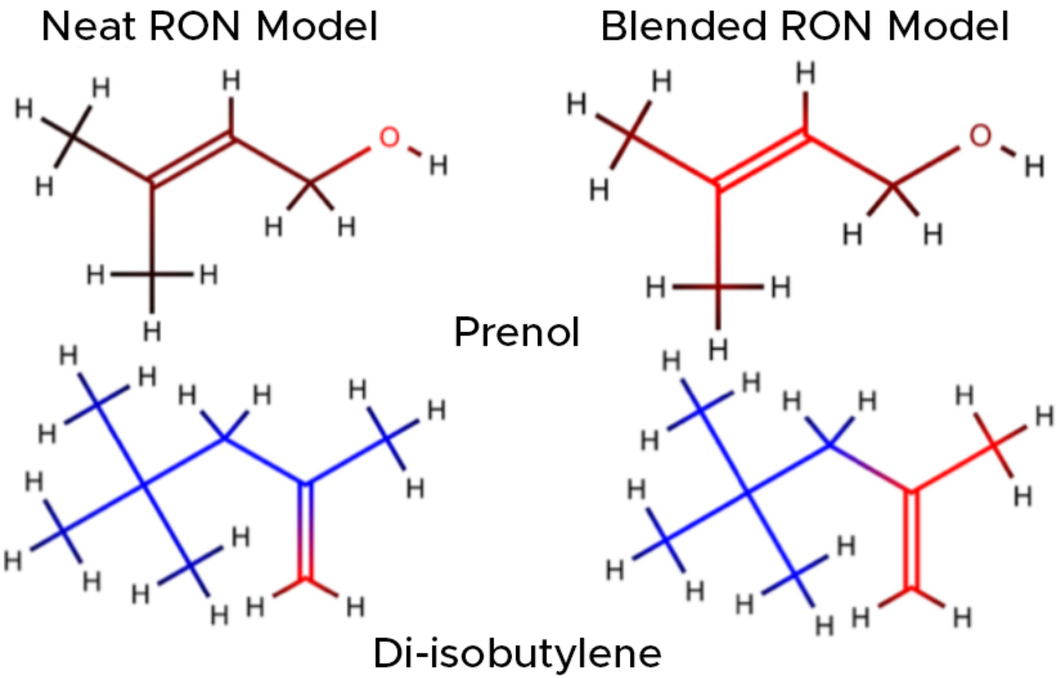




IMEP = indicated mean effective pressure, a measure of load

APPROACH Establish structure-property relationships

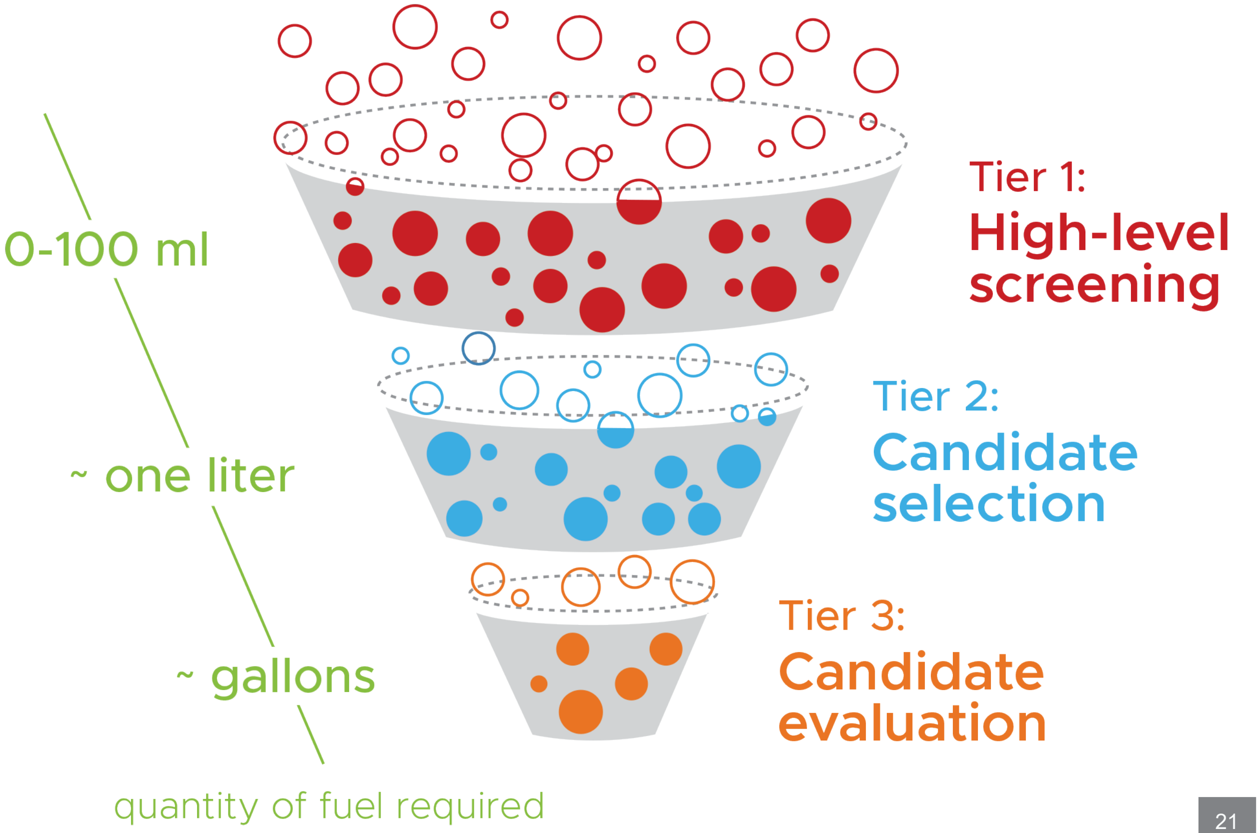
- Developed new tools linking chemistry to properties
- Identify candidate biofuels
- Some tools available to public



https://github.com/sandialabs/FeatureCreature

APPROACH Identify bioblendstocks

What biomass and waste-derived blendstocks contribute desired fuel properties?



0-100 ml

~ one liter

~ gallons

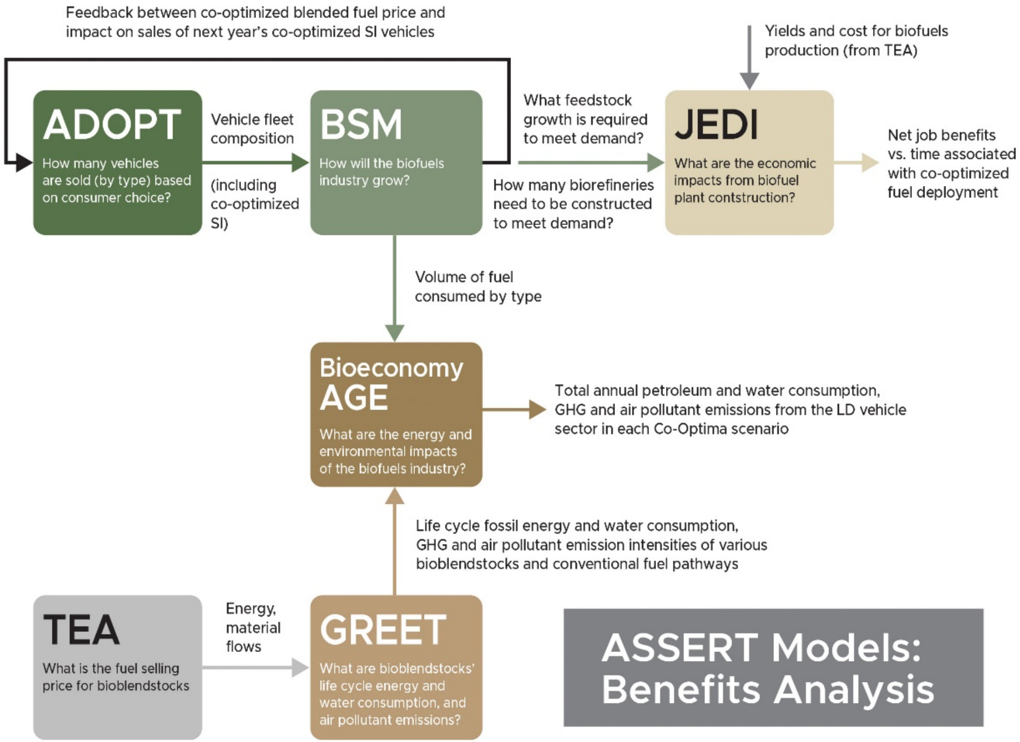
quantity of fuel required

Tier 1:
High-level screening

Tier 2:
Candidate selection

Tier 3:
Candidate evaluation

APPROACH Evaluate impacts



Feedback between co-optimized blended fuel price and impact on sales of next year's co-optimized SI vehicles

ADOPT

How many vehicles are sold (by type) based on consumer choice?

Vehicle fleet composition (including co-optimized SI)

BSM

How will the biofuels industry grow?

What feedstock growth is required to meet demand?

How many biorefineries need to be constructed to meet demand?

Yields and cost for biofuels production (from TEA)

JEDI

What are the economic impacts from biofuel plant contstruction?

Net job benefits vs. time associated with co-optimized fuel deployment

Volume of fuel consumed by type

Bioeconomy AGE

What are the energy and environmental impacts of the biofuels industry?

Total annual petroleum and water consumption, GHG and air pollutant emissions from the LD vehicle sector in each Co-Optima scenario

Life cycle fossil energy and water consumption, GHG and air pollutant emission intensities of various bioblendstocks and conventional fuel pathways

TEA

What is the fuel selling price for bioblendstocks

Energy, material flows

GREET

What are bioblendstocks' life cycle energy and water consumption, and air pollutant emissions?

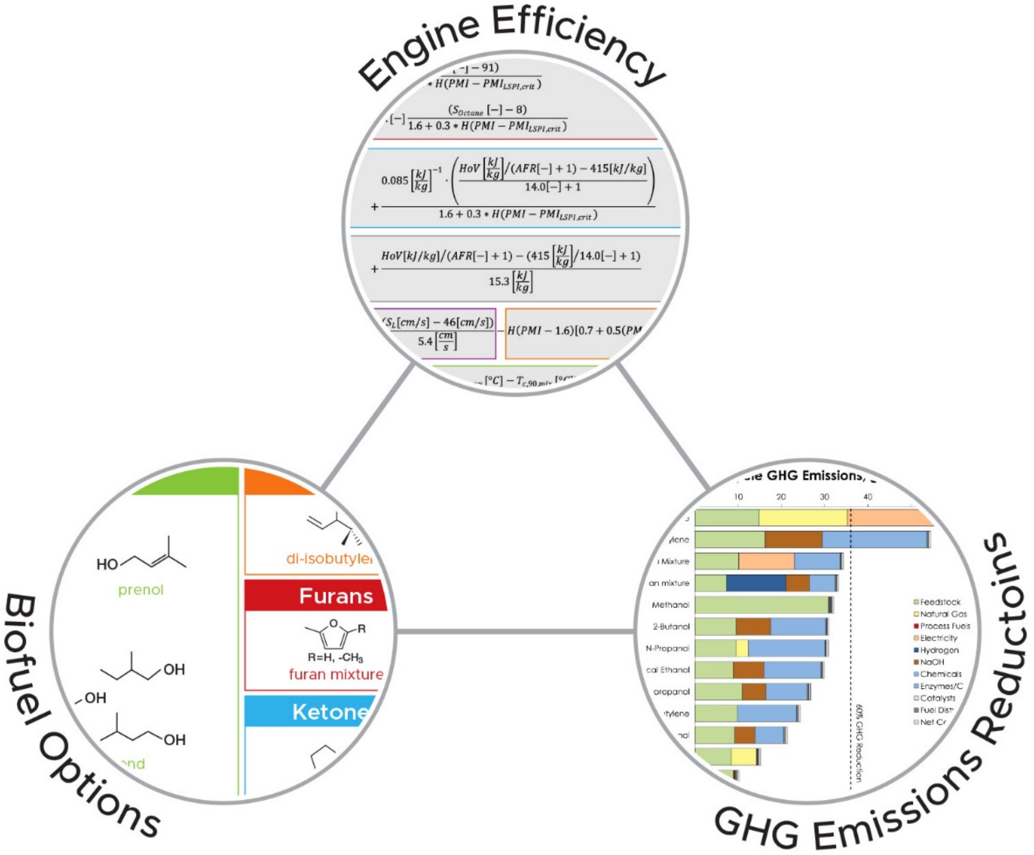
ASSERT Models: Benefits Analysis

- Techno-economic and wells-to-wheels life cycle analyses inform biofuel research
- Validated models linked by analysts to answer complex questions on impacts

Notable Outcomes

Fuel-engine co-optimization can achieve 10% efficiency gains

OUTCOMES Improving efficiency and reducing GHG



- Many blendstock options enable increased efficiency and reduced emissions
- Most important fuel properties – RON, S, HoV
- Durable methodology to guide future fuel development

OUTCOMES Merit function points way

$$Efficiency = 100 * \frac{\eta - \eta_{ref}}{\eta_{ref}}$$

$$= \frac{(RON[-] - 91)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})}$$

$$- K[-] \frac{(S_{Octane}[-] - 8)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})}$$

Octane Index Terms

$$+ \frac{0.085 \left[\frac{kJ}{kg}\right]^{-1} \cdot \left(\frac{HoV\left[\frac{kJ}{kg}\right]/(AFR[-] + 1) - 415[kJ/kg]}{14.0[-] + 1}\right)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})}$$

Heat of Vaporization on Knock Mitigation

$$+ \frac{HoV[kJ/kg]/(AFR[-] + 1) - \left(415\left[\frac{kJ}{kg}\right]/14.0[-] + 1\right)}{15.3\left[\frac{kJ}{kg}\right]}$$

Other Combined Heat of Vaporization

Flame Speed

$$+ \frac{(S_L[cm/s] - 46[cm/s])}{5.4\left[\frac{cm}{s}\right]}$$

$$- H(PMI - 1.6)[0.7 + 0.5(PMI - 1.4)]$$

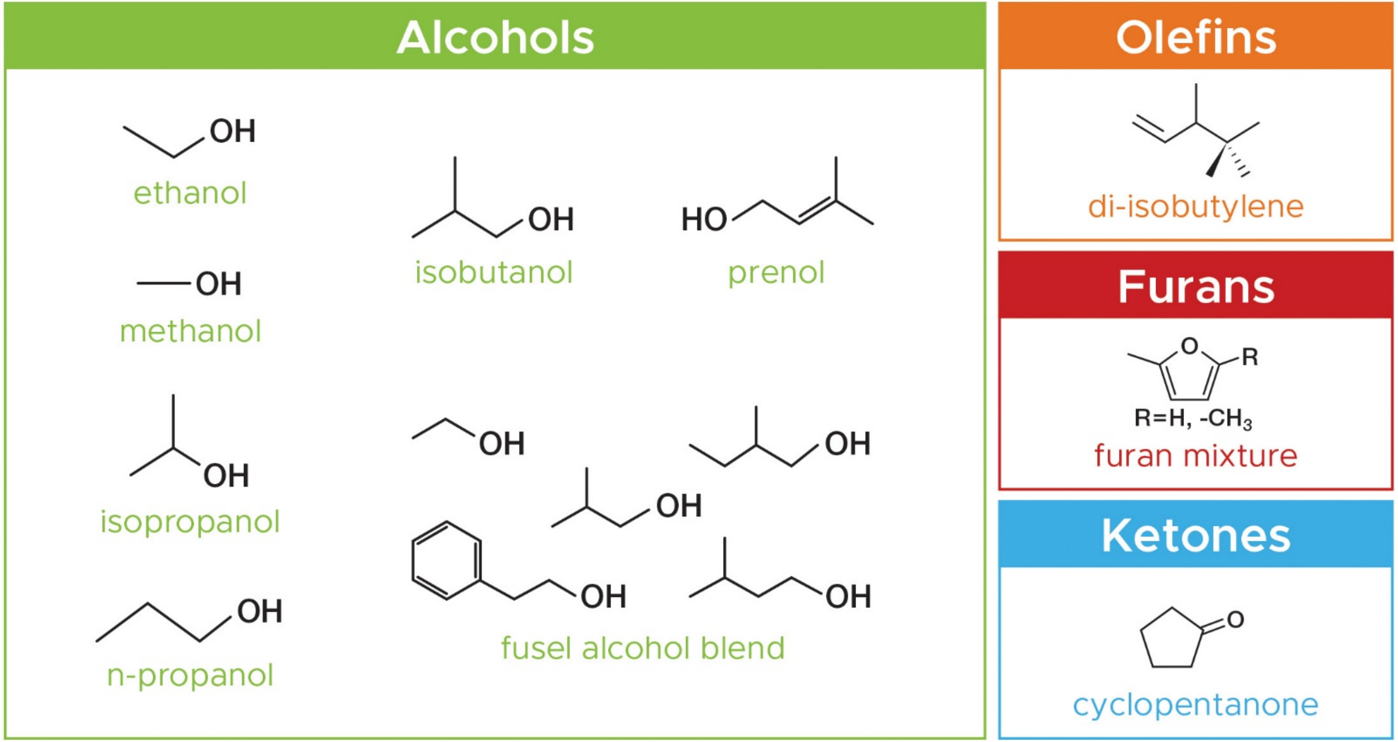
Particulate Emissions

$$+ 0.008[°C]^{-1}(T_{c,90,conv}[°C] - T_{c,90,mix}[°C])$$

Catalyst Light-Off

OUTCOMES Many blendstock options

- All have high RON, S
- Smaller alcohols also have high HoV
- RON for these blendstocks blend synergistically



Alcohols

ethanol

methanol

isobutanol

prenol

isopropanol

n-propanol

fusel alcohol blend

Olefins

di-isobutylene

Furans

$R=H, -CH_3$

furan mixture

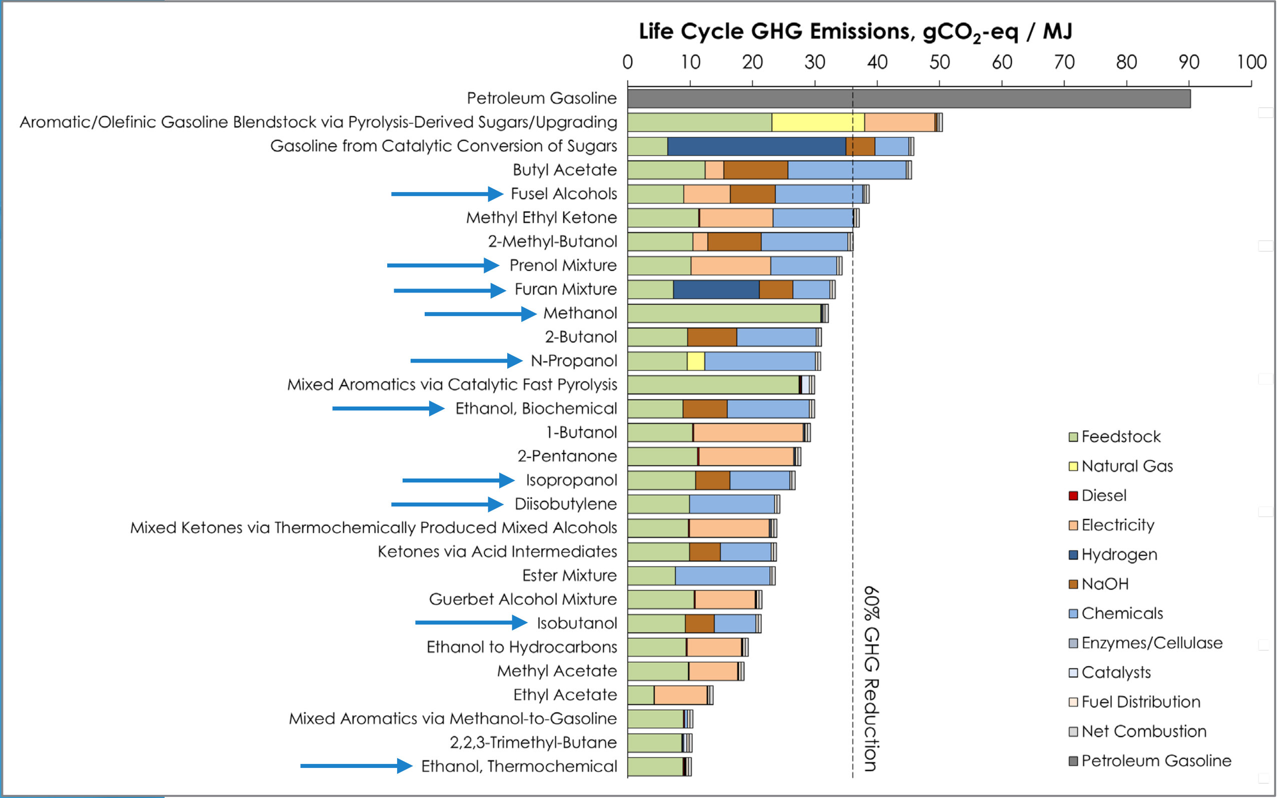
Ketones

cyclopentanone

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

OUTCOMES Biofuels reduce GHG emissions

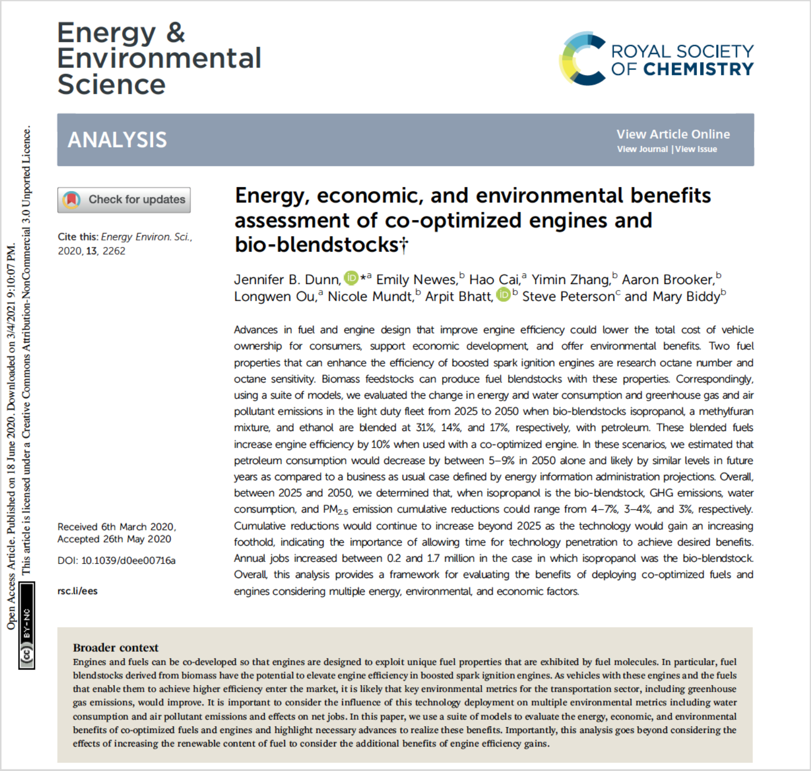
- Wide range of well-to-wheels GHG emissions reductions
- Top candidates all reduce GHG emissions by >50%
- Petroleum gasoline emissions are ~90 gCO_2 / MJ



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



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ROYAL SOCIETY
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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.

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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.

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Q & A

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