



Co-Optimization of  
Fuels & Engines

Octane and Internal Combustion  
Engine Advancements from a  
Long(er) Term Perspective:  
Insights from the Co-Optima Project  
Fuels2018

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May 22, 2018

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better fuels | better vehicles | sooner

U.S. DEPARTMENT OF  
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# The octane game: Auto industry lobbies for 95 as new regular

April 17, 2018 @ 11:00 am

419

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GM, Ford and Fiat Chrysler are seeking just one grade of fuel: 95. That would eliminate today's grades, generally 87 octane for regular, 88-90 for midgrade and 91-94 for premium. Photo credit: BLOOMBERG

## Related Stories



**New 1.5-liter Ford engine can run on just 2 cylinders**

UPDATED: 4/18/18 11:06 am ET - [adds details](#)

The auto industry is finally getting traction on its quest to make 95 RON octane gasoline -- basically the same grade as Europe's regular and the lowest grade of premium here -- the new regular in the United States.

In **testimony** Friday before the House Energy and Commerce Committee's environment

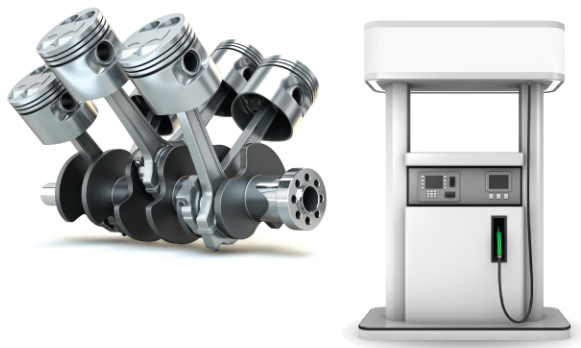
subcommittee, Dan Nicholson, General Motors'

vice president of global propulsion systems, said making 95 octane the new regular aligns the U.S. with Europe and is one of the most affordable ways to boost fuel economy and lower greenhouse gas emissions.

# Key Takeaway Messages



**ICEs and liquid fuels**  
will be around a long time



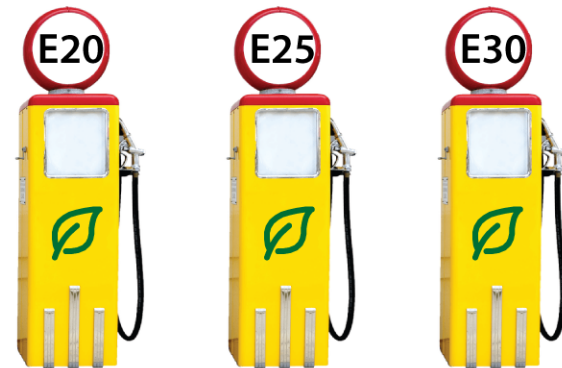
And their efficiency/emissions can be improved significantly

**95 RON**  
is directionally a good start  
for boosted SI engines



But we need to consider octane sensitivity/other properties and advanced engine needs

**Ethanol**  
is one viable path to  
high RON, lower GHG fuels



But other bio-blendstocks could provide additional longer-term options/flexibility

**Goal:** better  
fuels and  
better vehicles  
**sooner**



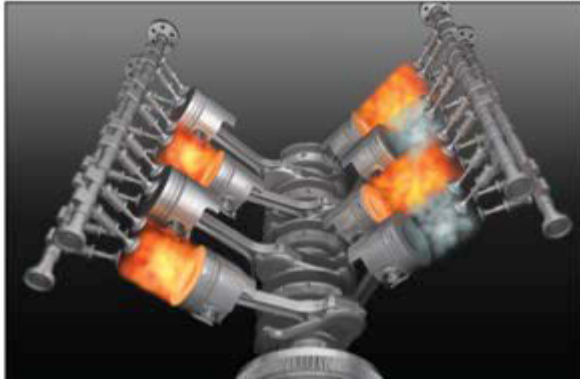
## Fuel and Engine Co-Optimization

- What fuel properties maximize engine performance?
- How do engine parameters affect efficiency?
- What fuel and engine combinations are sustainable, affordable, and scalable?

# Key Co-Optima Research Questions



What fuels do  
engines  
*really* want?



What fuels  
*should* we make?



What will work  
in the real world?



# Two Parallel R&D Projects



## Light-Duty



Boosted SI

Higher efficiency  
via downsizing

Near-term



Multi-mode SI/ACI

Even higher efficiency  
over drive cycle

Mid-term

## Medium/Heavy-Duty



Mixing Controlled

Improved engine  
emissions

Near-term



Kinetically  
Controlled

Highest efficiency and  
emissions performance

Longer-term

# High-level goals and outcomes



## Light-duty

10% fuel economy (FE) improvement\* from boosted SI and multi-mode SI/ACI

## Heavy-duty

Up to 4% FE improvement (worth \$5B/year)\*  
Potential lower cost path to meeting next tier of criteria emissions regulations

## Fuels

Diversifying resource base

Providing economic options to fuel providers to accommodate changing global fuel demands

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

## Cross-cutting goals

Stimulate domestic economy

Adding up to 500,000 new jobs

Providing clean-energy options

\* Beyond projected results of current R&D efforts; 2030 target. The team is actively engaging with OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring fuel economy improvements

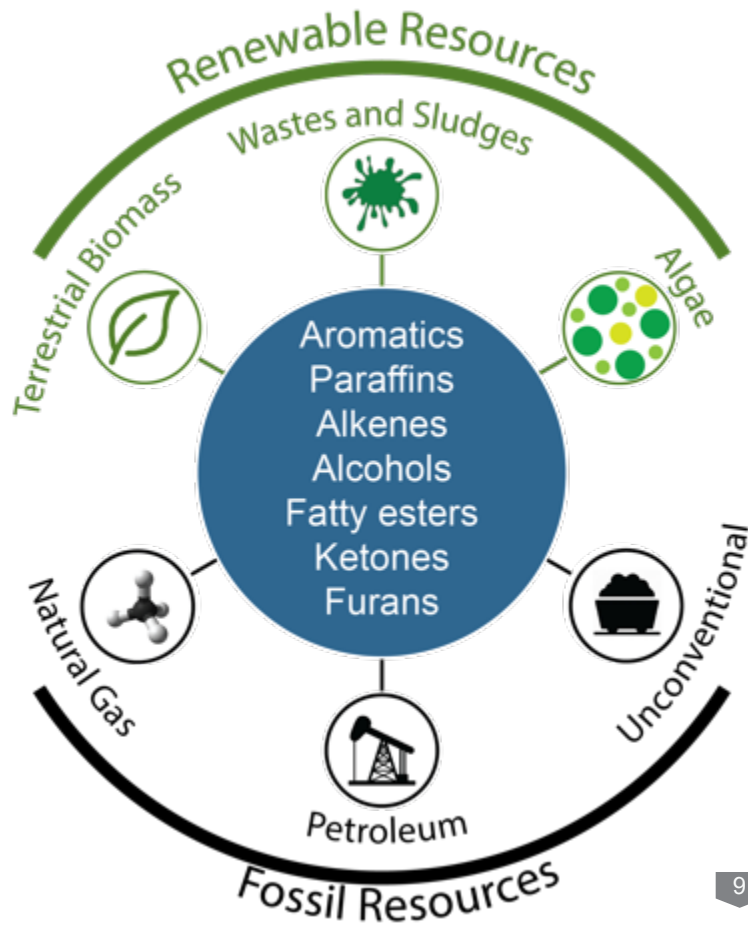


# Approach



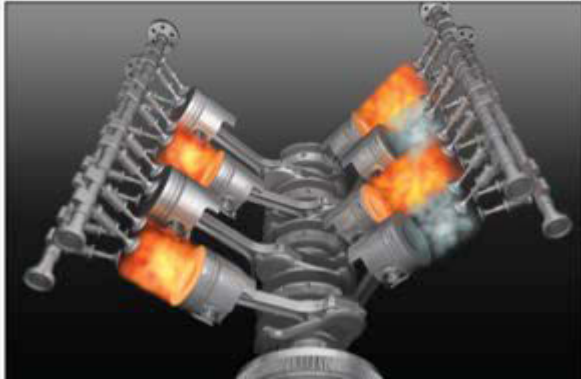
Objective: identify fuel properties that optimize engine performance, independent of composition,\* allowing the market to define the best means to blend and provide these fuels

\* We are not going to recommend that any specific blendstocks be included in future fuels





What fuels do  
engines  
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# Question 1: What fuels do engines really want?



## Approach:

Conduct engine experiments and simulations that delineate fuel property impacts on engine performance

Focus: boosted SI engines

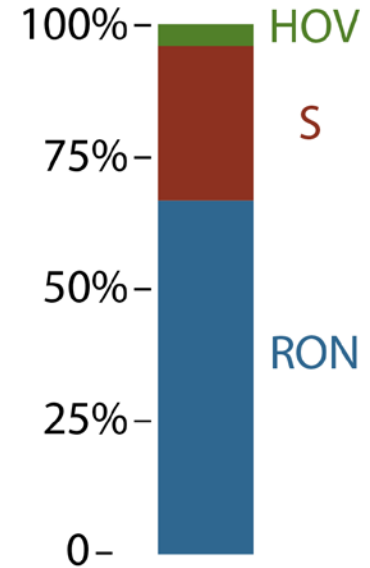


# Fuel Properties Impacting Boosted SI Efficiency

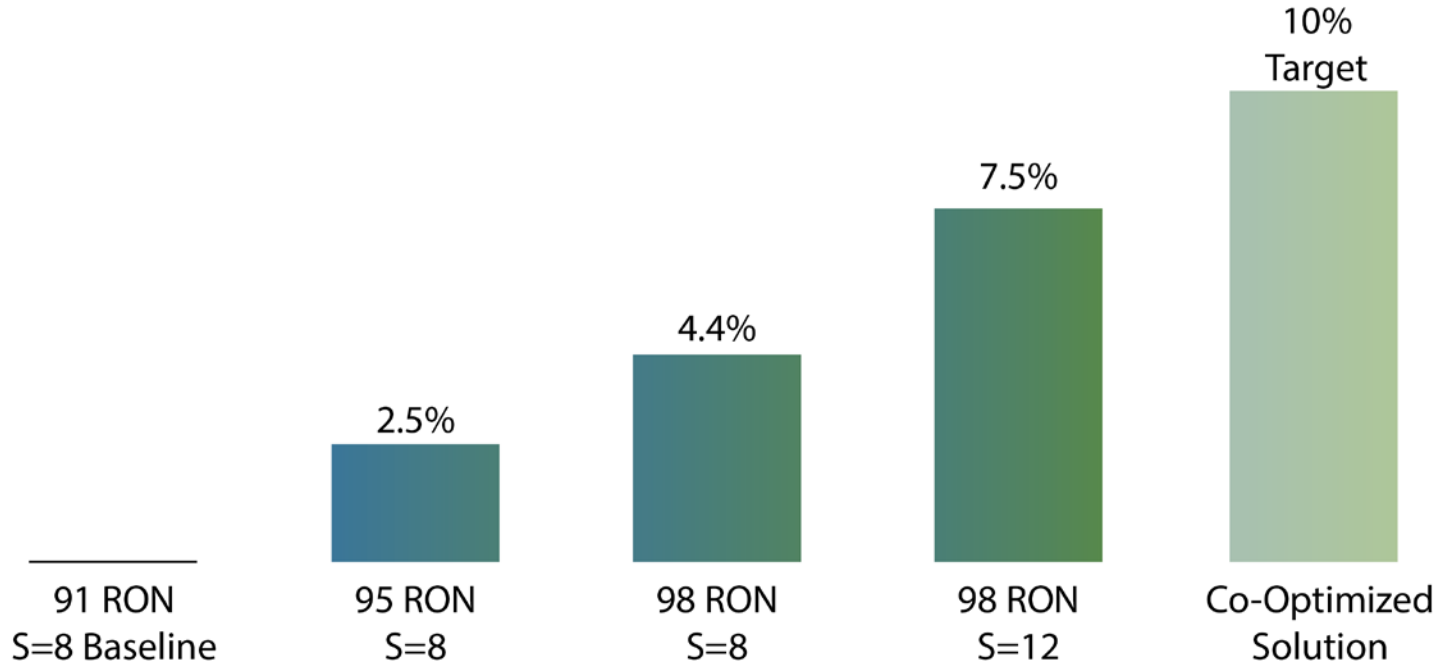


$$\begin{aligned}
 \text{Merit (efficiency)} = & \underbrace{\alpha \cdot f(\text{RON})}_{\text{Octane Index (Knock)}} + \underbrace{\beta \cdot f(K, S)}_{\text{Octane Sensitivity}} + \underbrace{\gamma \cdot f(\text{HOV})}_{\text{Charge Cooling}} \\
 & + \underbrace{\varepsilon \cdot f(\text{LFS})}_{\text{Burn Rate/ Dilution Tolerance}} + \underbrace{\zeta \cdot f(\text{PMI})}_{\text{PM Emissions}} + \underbrace{\eta \cdot f(T_{c,90,conv})}_{\text{Catalyst Light-off Temp (cold start)}}
 \end{aligned}$$

Average contribution to merit function for highest scoring blendstocks



# Efficiency Improvement: Boosted SI Engines



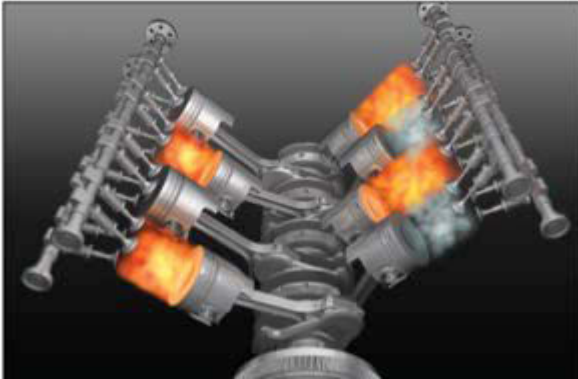
S = sensitivity = RON - MON; Engine efficiencies calculated for conditions appropriate for boosted downsized engines ( $K = -1.25$ )

Source: Miles, Paul. "Efficiency Merit Function for Spark Ignition Engines: Revisions and Improvements Based on FY16-17 Research." Technical Report. U.S. Department of Energy, Washington, DC. 2018. DOE/GO-102018-5041.

# Foundational Technical Questions



What fuels do  
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What fuels  
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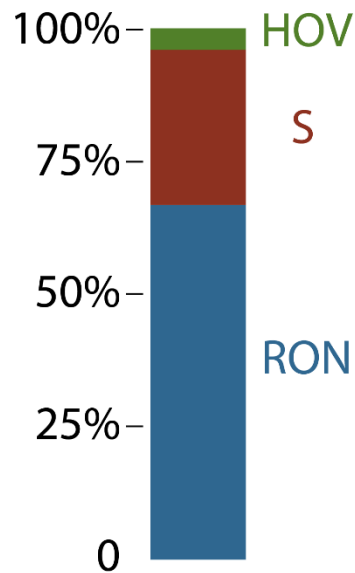
What will work  
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# Current Boosted SI Blendstock Evaluation



Average contribution to merit function for highest scoring blendstocks



Properties provided by chemical families:

	RON	S	HOV
Alcohols	✓	✓	✓
Furans	✓	✓	
Alkenes	✓	✓	
Aromatics	✓	✓	
Ketones	✓	✓	
Cycloalkanes	✓	✓	
Esters	✓	✓	
Alkanes	✓		
Ethers	✓		

Blendstocks from 5 chemical families selected for more detailed evaluation

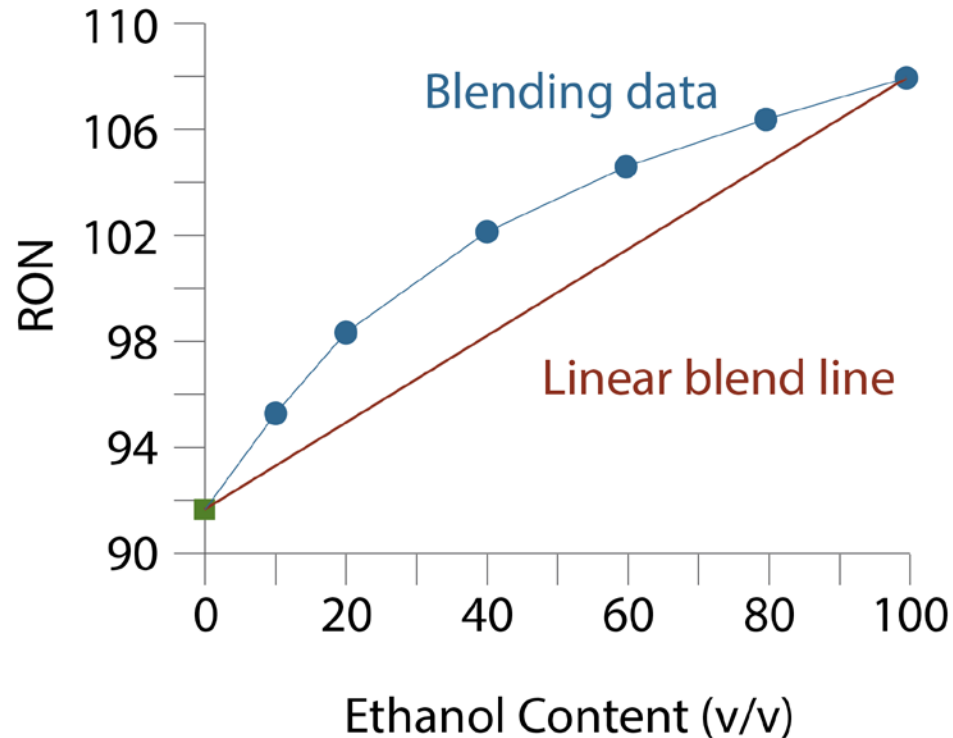
Alcohols	
<chem>CCO</chem> ethanol	<chem>CCCO</chem> n-propanol
<chem>CC(C)O</chem> isopropanol	<chem>CC(C)CO</chem> isobutanol
Ketones	Olefins
<chem>C1CCCC1=O</chem> cyclopentanone	<chem>CC(C)=CC</chem> di-isobutylene
Furans	Aromatics
<chem>C1=CC=C(O1)R</chem> R = H, -CH <sub>3</sub> furan mixture	<chem>C1=CC=CC=C1R</chem> aromatic mixture

RON = Research octane number ; S = Sensitivity (S = RON - MON) ; HOV = heat of vaporization

# Understanding Blending Effects

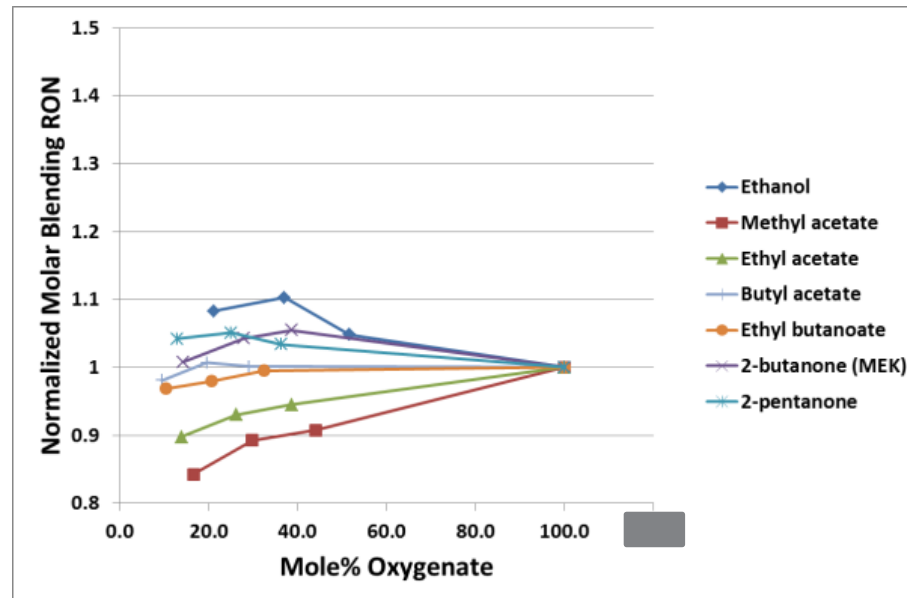
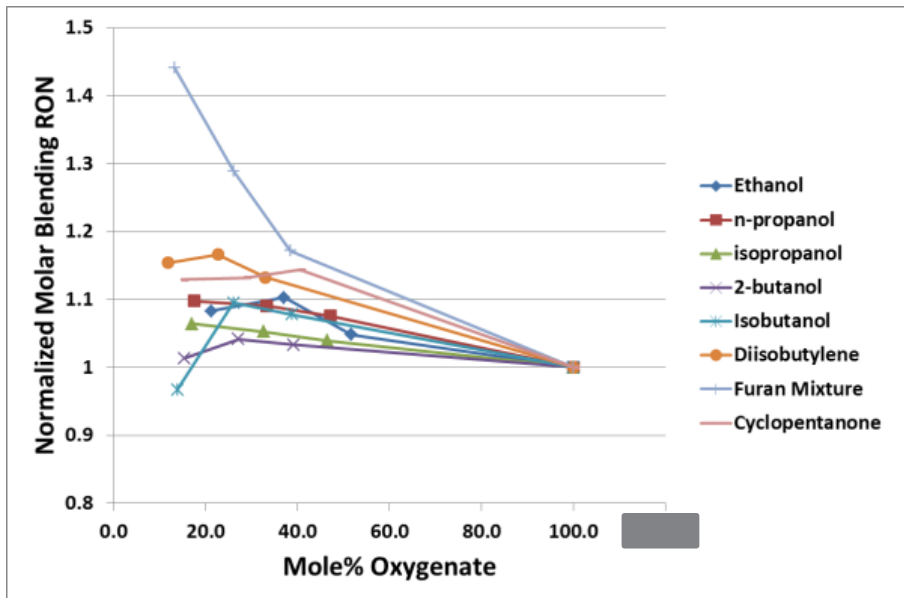


- Many blendstocks exhibit beneficial non-linear blending behavior
  - “Effective” blending number is higher than pure component’s
- Value proposition:
  - Determine molecular basis for non-linear RON and S blending
  - Identify blendstocks with greatest potential to impart advantageous properties





# RON Blending Behavior



- Comprehensive blending studies in gasoline surrogate w/ and w/o ethanol
- Non-linear blending is norm
  - May be either synergistic (furans) or antagonistic (esters)

# Capitalizing on Synergistic Blending



## Blendstock volumes required to produce 95 RON fuel from 88 RON BOB

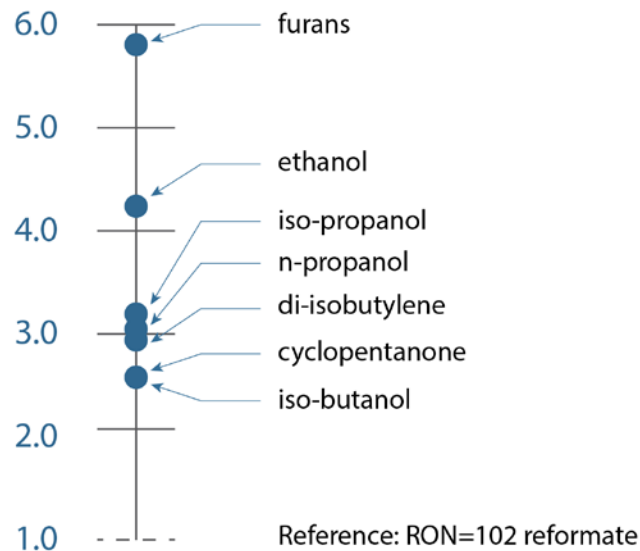
	Blendstock (vol)	88 RON BOB (vol)
furans	0.09	0.91
ethanol	0.12	0.88
iso-propanol	0.16	0.84
n-propanol	0.17	0.83
di-isobutylene	0.17	0.83
iso-butanol	0.19	0.81
cyclopentanone	0.19	0.81
reformate (RON=102)*	0.50	0.50

In this BOB, furans are 5.8x as effective on a volumetric basis than reformate

\* reference

Four-component surrogate BOB; Blending data from: R.L. McCormick et al., SAE Int. J. Fuels Lubr., 10:442-460, 2017.

## Performance-based volume parity factor for producing 95 RON fuel

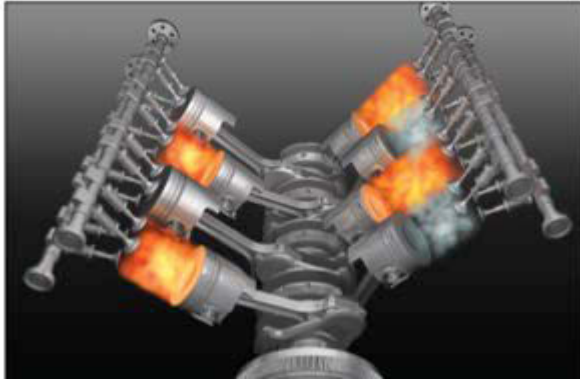


Thus, furans can be more expensive than reformate (per gallon) and provide a more affordable option for consumers

# Foundational Technical Questions



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# The Role of Analysis in Co-Optima



## Bioblendstock Level



What are the scalability, cost, and environmental drivers?

Is a given bio-blendstock viable in the near term?

What are the key research challenges that must be overcome?

## Transportation Sector Level



What will be the influence on fleet:

- Energy consumption
- Emissions – air pollutants, GHG
- Water consumption

What are potential impacts on infrastructure?

## Feedstock Supply



How can companion markets build feedstock supply and what will be price impact?

## Refinery Integration



What would the value proposition be to a refiner for integrating a certain bioblendstock?

# Goal: Identify Key Bioblendstock Research Challenges



## Technology Readiness

State of technology:  
Fuel production

State of technology:  
Vehicle use

Conversion technology  
readiness level

Feedstock sensitivity

Process robustness

Feedstock quality

# of viable pathways



## Environmental

Carbon efficiency

Target yield

Life cycle greenhouse  
gas emissions

Life cycle water

Life cycle fossil  
energy use



## Economics

Target cost

Needed cost reduction

Co-product economics

Feedstock cost

Alternative high-value  
use



## Other Factors

Regulatory requirements

Geographic factors

Vehicle compatibility

Infrastructure  
compatibility

Assessed only for blendstocks  
produced from biomass

Assessed for both fossil  
and renewable blendstocks

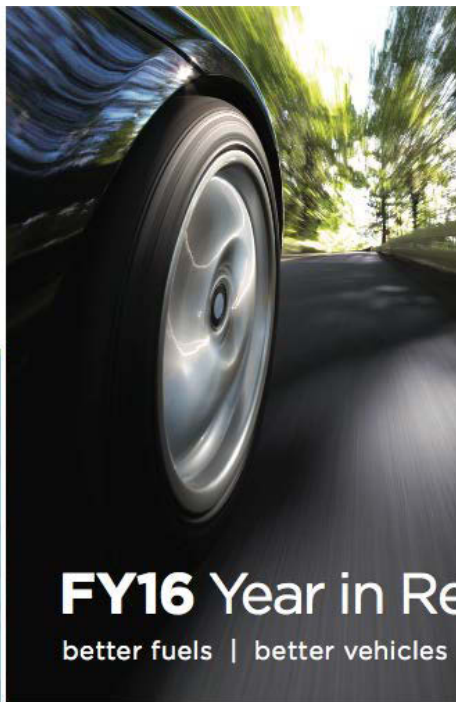


- Co-Optima research and analysis have identified fuel properties that enable advanced LD and HD engines
  - 95 RON will directionally improve boosted SI efficiency, but higher RON and S provide additional benefits
  - The optimal fuel properties for future engines are still uncertain
- There are a large number of blendstocks readily derived from biomass (and petroleum) that possess beneficial properties
  - Some may provide longer term options in addition to ethanol
- Key research needs have been identified for performance, technology, economic, and environmental metrics

# More Info Available



Co-Optimization of  
Fuels & Engines



**FY16** Year in Review  
better fuels | better vehicles



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Thank You!