Co-Optimization of Fuels & Engines

Fuel Properties for Advanced Spark Ignition Engines: Insights from the U.S. DOE Co-Optima Project

The International Summit on Breakout Technologies of Engine and Fuel (ISEF2018)

John Farrell, National Renewable Energy Lab

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Acknowledgments

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Co-Optima Technical Team Leads:

Anthe George (SNL), Paul Miles (SNL), Jim Szybist (ORNL),
Jennifer Dunn (ANL), Matt McNenly (LLNL)

Co-Optima Leadership Team:

John Farrell (NREL), Robert Wagner (ORNL),
Chris Moen (SNL), Dan Gaspar (PNNL)

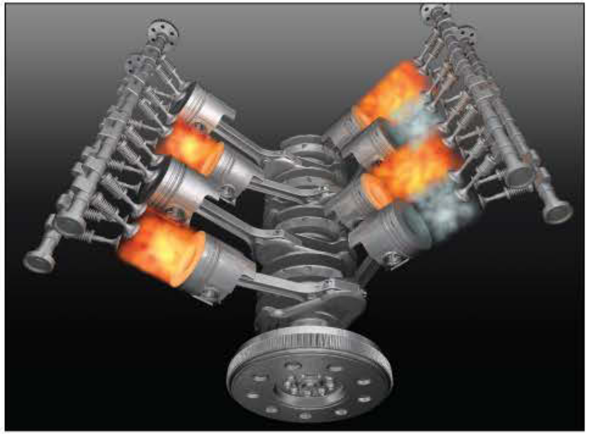
Goal: better fuels and better vehicles **sooner**

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?

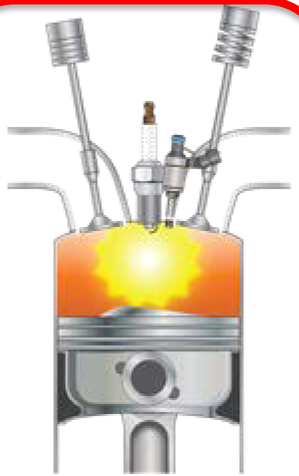


What fuel options work best?

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

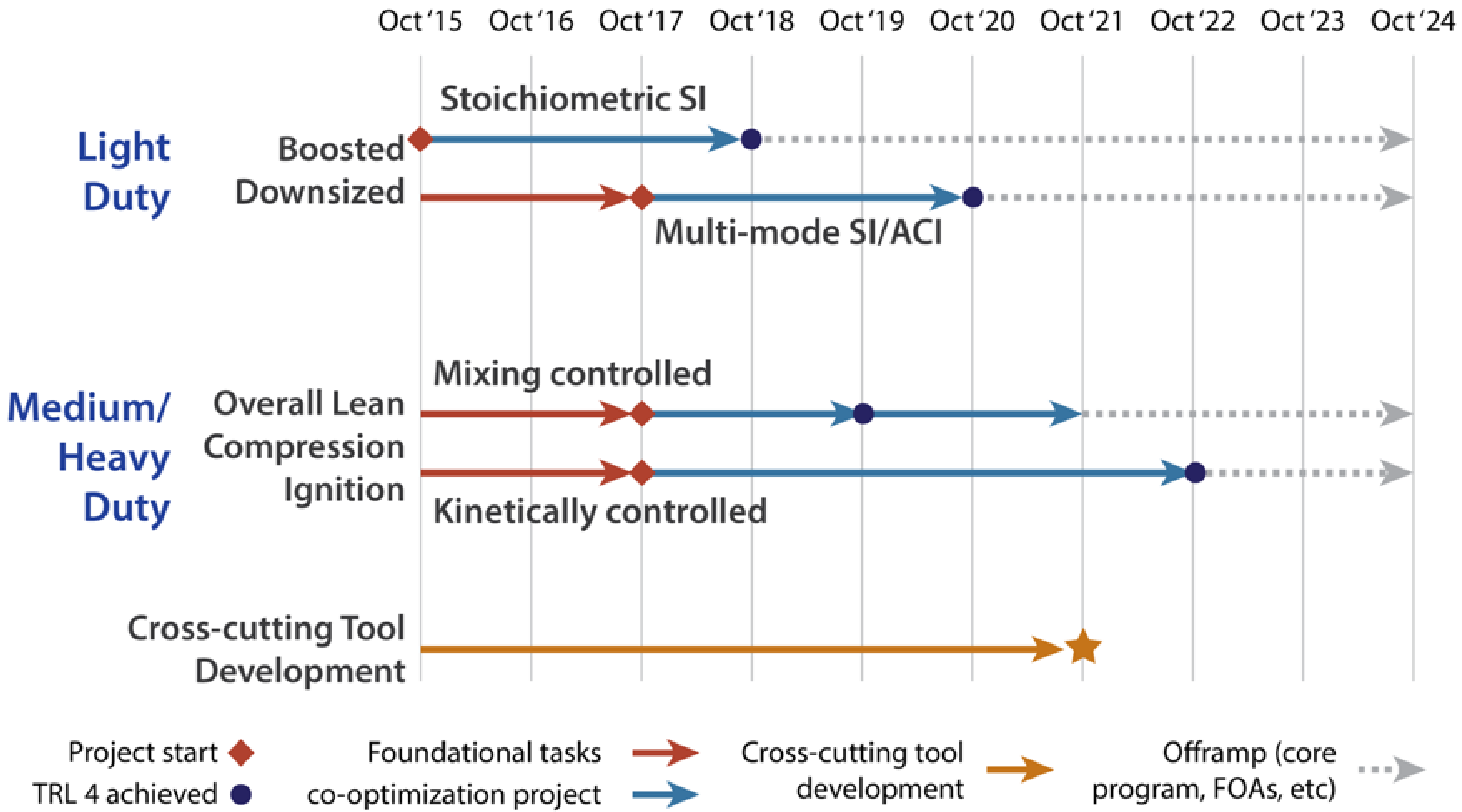
Near-term

Kinetically Controlled

Highest efficiency and emissions performance

Longer-term

Project Timeline



High-level goals and outcomes

Light-duty

35% 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

Identify fuel blendstocks with significantly lower well-to-wheel GHG emissions

Diversify resource base

Provide economic options to fuel providers to accommodate changing global fuel demand

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

Cross-cutting goals

Stimulate domestic economy

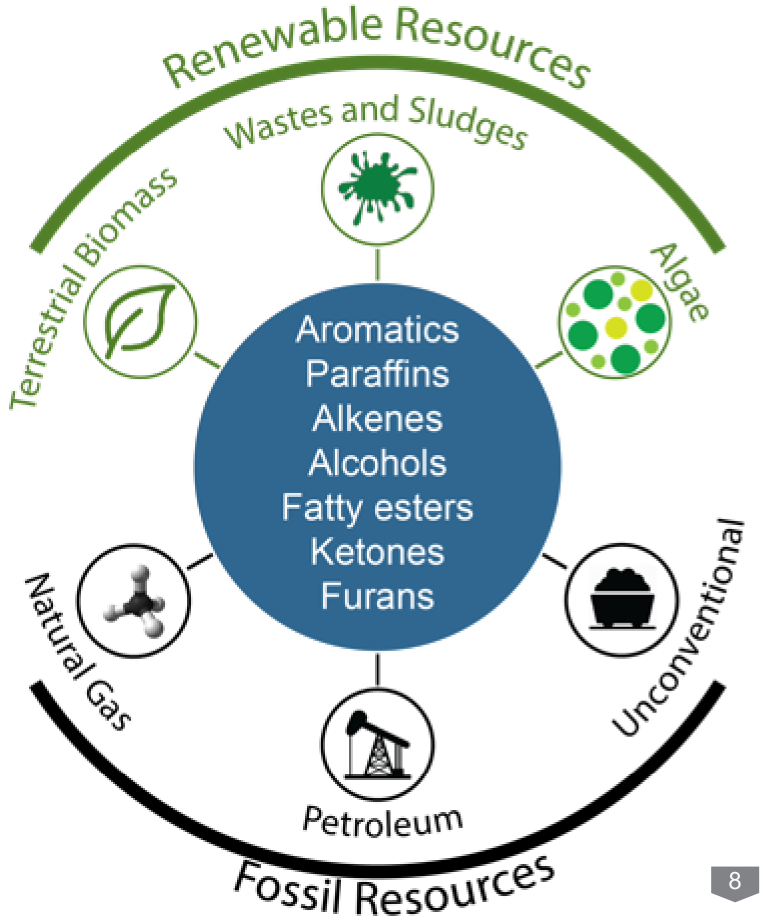
Provide clean-energy options

* vs. 2015 reference case; 2030 target. 25% comes from base engine and 10% from fuel/engine co-optimization
** Beyond projected results of current R&D efforts; 2030 target.

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



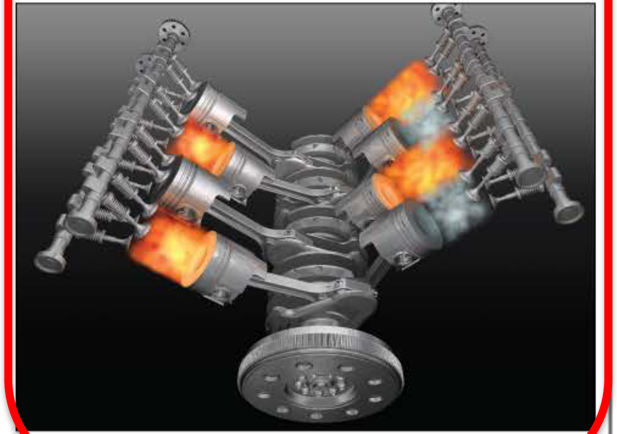
Brings Together National Leadership and Expertise

Team:

- 9 national laboratories
- 13 universities
- An open funding opportunity in FY 2018 will bring in additional university and industry partners

Foundational Technical Questions

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

Question 1: What fuels do engines really want?

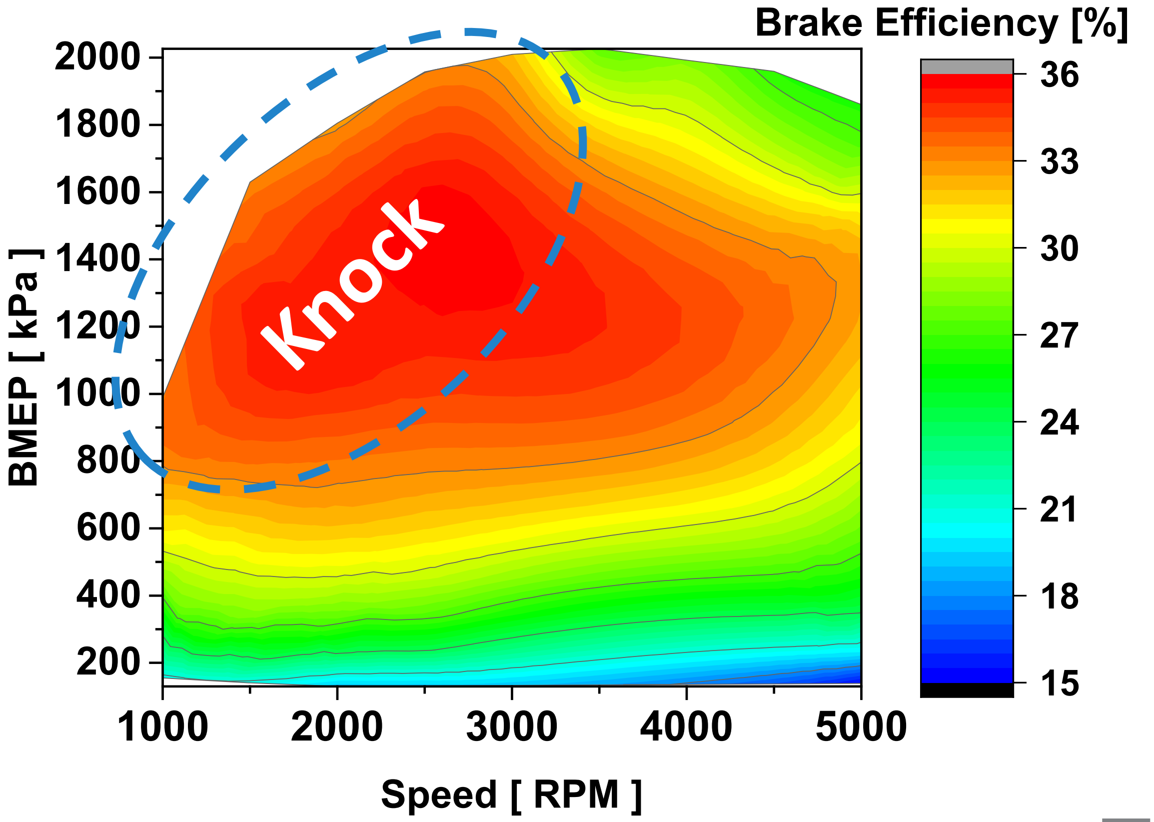
Approach:

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

Focus: boosted SI engines

What Limits Engine Efficiency?

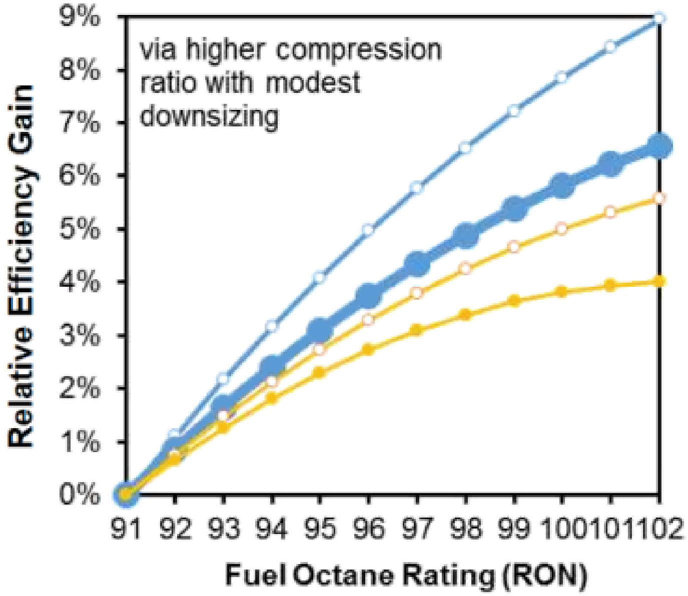
- Engines are most efficient at high load, low speed
- These are also conditions that exacerbate knock and limit efficiency
- Fuels with high octane number (RON/MON) are able to mitigate knock, providing higher efficiency



Engine Efficiency from Higher Octane Fuel (HOF)

USCAR Model*

Higher fuel octane rating (RON) → Raise compression ratio (CR) → Improve efficiency

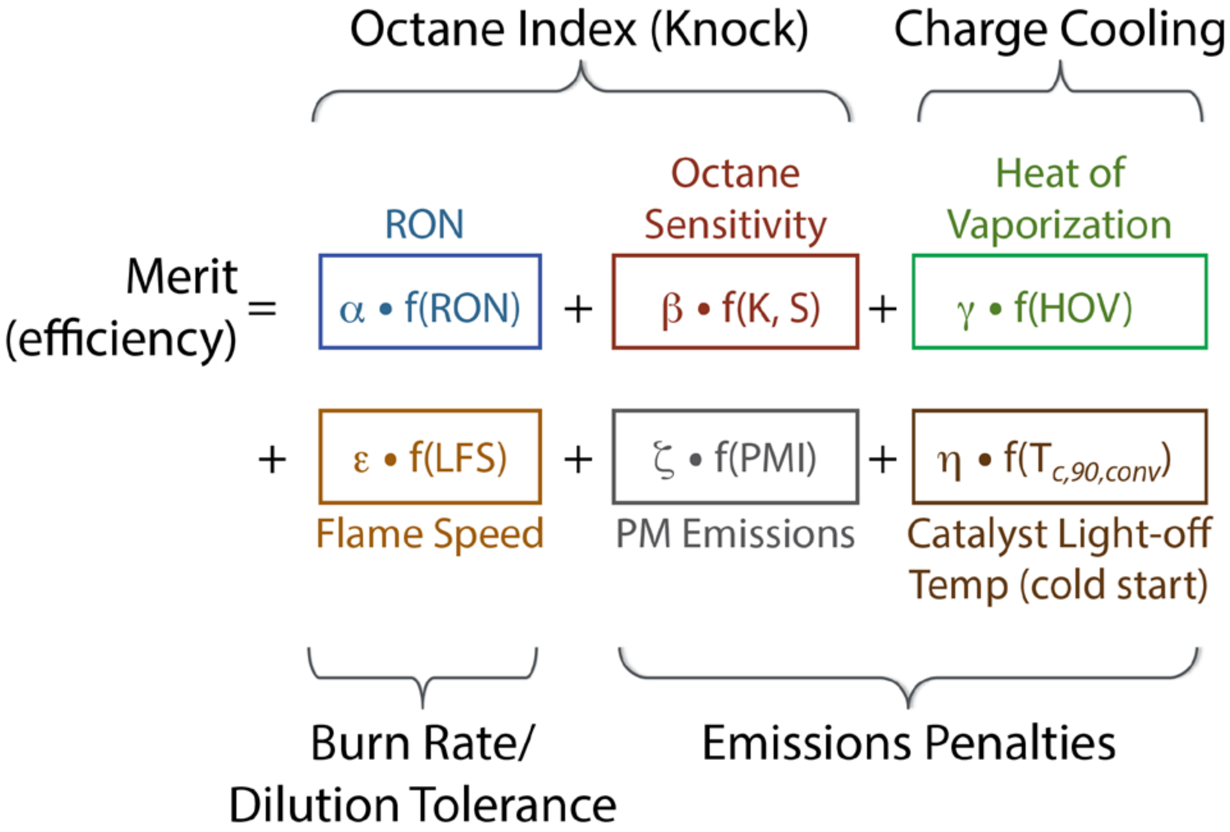


Slide information taken from USCAR presentation in Jan 2018

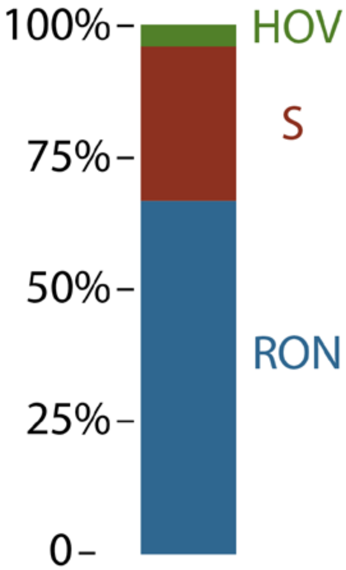
* Citation:
Leone, Anderson, Davis, Iqbal, Reese, Shelby, and Studzinski, "The Effect of Compression Ratio, Fuel Octane Rating, and Ethanol Content on Spark-Ignition Engine Efficiency", Environmental Science & Technology 2015.

HOF enables efficiency increases for all vehicles with SI engines including hybrid electric vehicles

Fuel Properties Impacting Boosted SI Efficiency



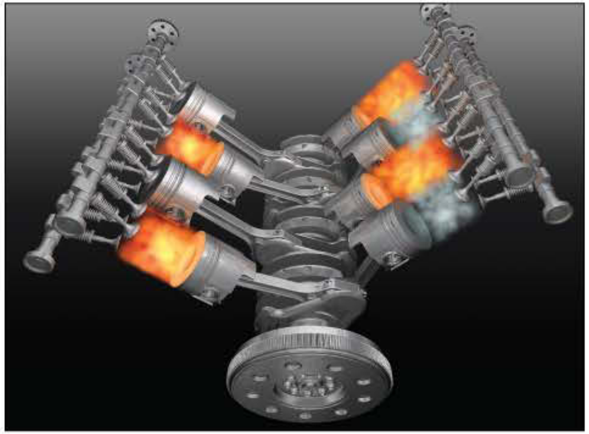
Average contribution to merit function for highest scoring blendstocks



https://www.energy.gov/sites/prod/files/2018/02/f48/Co-Optima%20Merit%20Function%20Report%2067584_2.pdf

Foundational Technical Questions

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

Initial Boosted SI Blendstock Evaluation (2017)

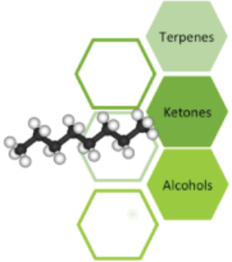
Rigorous Screening

Rapidly identify viable candidates

Blendstock Evaluation

Measure properties

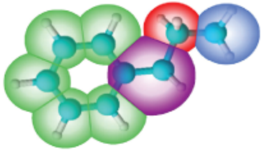
Populate database

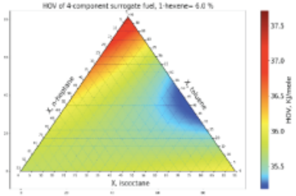


Generate Insight

Develop blending models

Correlate properties to molecular structure

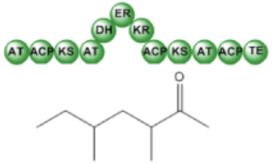




Establish Bio Pathways

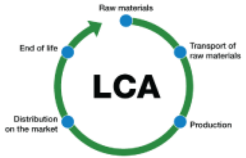
Target properties to generate key data

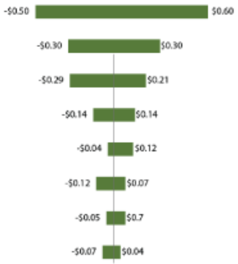
Conduct retrosynthetic analyses



Inform Analyses

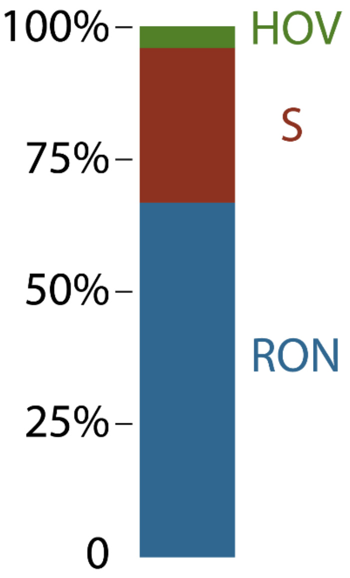
Provide improved data for LCA, TEA analyses





Initial Boosted SI Blendstock Evaluation (2017)

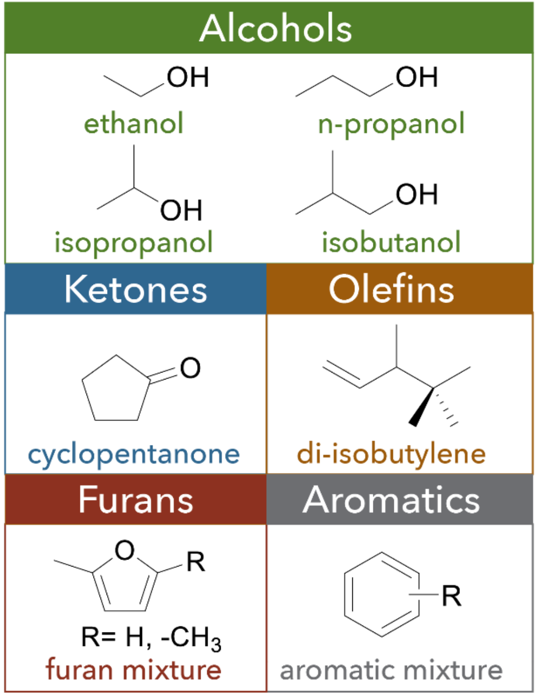
Average contribution to efficiency merit function for highest scoring blendstocks



Properties provided by chemical families:

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

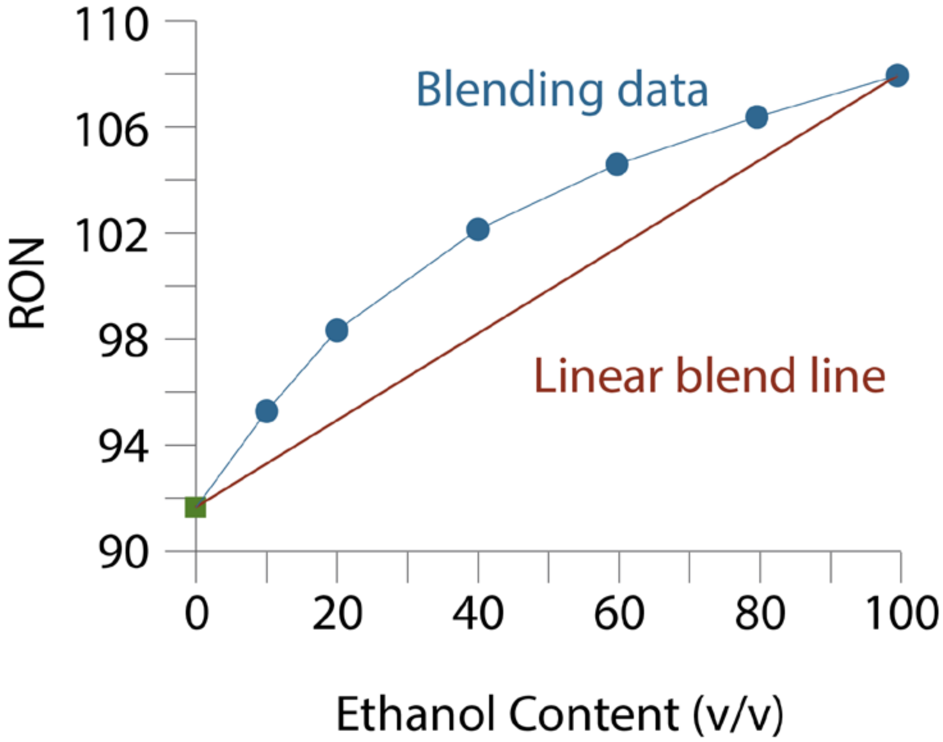
Blendstocks from 5 chemical families selected for more detailed evaluation



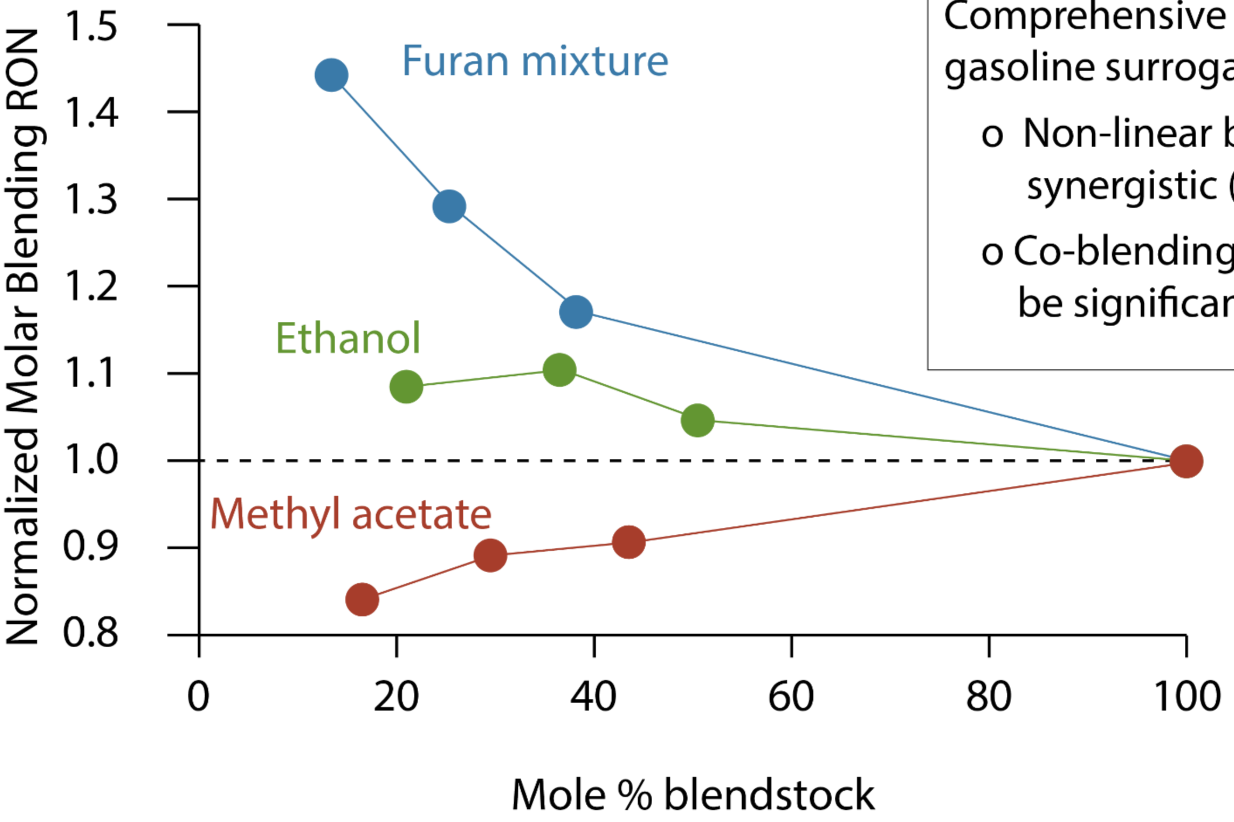
RON = Research octane number ; S = Sensitivity (S = RON – MON) ; HOV = heat of vaporization

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 carried out in gasoline surrogate w/ and w/o ethanol

- Non-linear blending is typical; may be synergistic (furans) or antagonistic (esters)
- Co-blending interactions with ethanol can be significant (i.e., non-linearity is different)

Capitalizing on Synergistic Blending

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

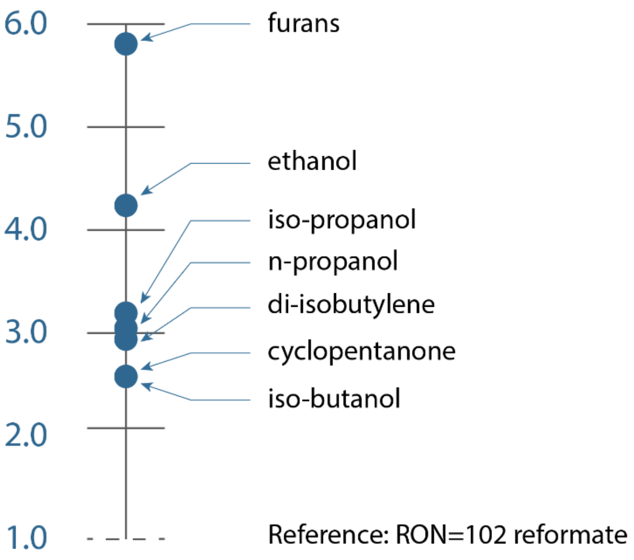
	Blendstock (vol)	88 RON BOB (vol)
furans	0.09	0.91
ethanol	0.12	0.88
iso-propanol	0.16	0.84
n-propanol	0.17	0.83
di-isobutylene	0.17	0.83
iso-butanol	0.19	0.81
cyclopentanone	0.19	0.81
reformate (RON=102)*	0.50	0.50

In this BOB, furans are 5.8× 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

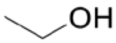


Thus, furans can be more expensive than reformate (per gallon) and provide a more affordable option for consumers

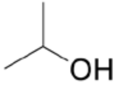
Current Boosted SI Blendstock Evaluation

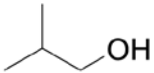
Preliminary (2017) list of blendstocks selected for more detailed evaluation

Alcohols

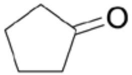

ethanol


n-propanol

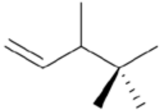

isopropanol


isobutanol

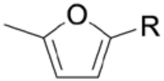
Ketones


cyclopentanone

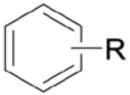
Olefins


di-isobutylene

Furans


R= H, $-CH_3$
furan mixture

Aromatics

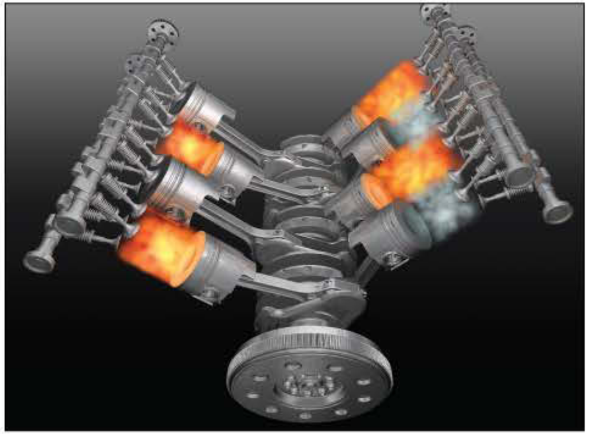

aromatic mixture

Final list of boosted SI blendstocks being developed (to be finalized end of FY18)

Alcohols	TBD
Ketones	TBD
Olefins	TBD
Esters	TBD
Furans	TBD
Aromatics	TBD

Foundational Technical Questions

What fuels do engines *really* want?



What fuel options work best?

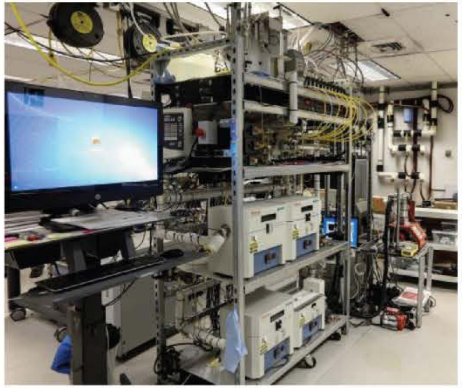
What will work in the real world?

Goal: identify key vehicle/infrastructure constraints

Low-speed preignition

Screen blendstocks to ensure no adverse propensity for LSPI

Emissions control



Identify aftertreatment impacts (oxidation, PM, NOx, toxics, etc.)

Materials compatibility

Screen for impacts on plastics, elastomers, and metals used in vehicles and infrastructure

Analysis answers key questions to inform R&D

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	Environmental	Economics	Other Factors
State of technology: Fuel production	Carbon efficiency	Target cost	Regulatory requirements
State of technology: Vehicle use	Target yield	Needed cost reduction	Geographic factors
Conversion technology readiness level	Life cycle greenhouse gas emissions	Co-product economics	Vehicle compatibility
Feedstock sensitivity	Life cycle water	Feedstock cost	Infrastructure compatibility
Process robustness	Life cycle fossil energy use	Alternative high-value use	
Feedstock quality			
# of viable pathways			

Technology Readiness, Environmental, Economics: Assessed only for blendstocks produced from biomass

Other Factors: Assessed for both fossil and renewable blendstocks

Key Analysis Takeaways

Feedstock Considerations

With sufficient availability and reasonable costs, feedstock issues do not impede successful deployment of biorefineries

Evolution of companion markets can support the overall feedstock market.

Key Analysis Takeaways

Process Considerations

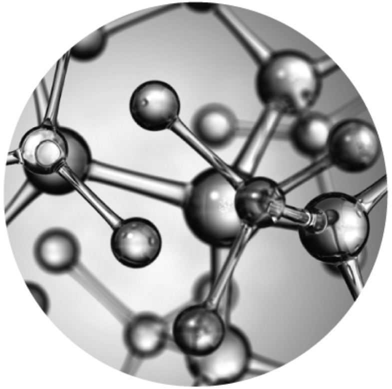
Yields in biochemical, sugar-based routes may be relatively lower than in thermochemical processes due to lower lignin utilization

Some biochemical process yields would see economic and environmental gains with improved microbial pathways

Catalyst lifetime/selectivity improvements are key to improving performance of thermochemical processes

Data regarding biofuel process conditions, yields, and selectivities are limited and ongoing analysis is needed to evaluate economic, environmental, and scalability of various biofuels

Key Analysis Takeaways



Fuel Property Considerations

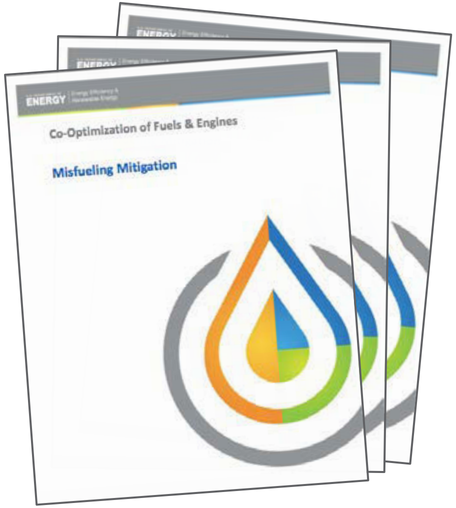
A more detailed understanding of structure/property relationships is needed to help guide process development

Better definition of required purity levels is needed to assess economic/environmental performance of thermochemical routes

Blending interactions are BOB-dependent and significantly impact blendstock volume requirements/economic targets

More Info Available

- Leading scientific journals
- Technical conferences
- DOE reports
- Annual Merit Review presentations
- Annual year-in-review summary documents



https://www.energy.gov/eere/vehicles/annual-merit-review
https://www.nrel.gov/docs/fy17osti/67595.pdf
https://www.energy.gov/sites/prod/files/2018/04/f50/Co-Optima_YIR2017_FINAL_Web_180417_0.pdf

Summary and Next Steps

Summary

- Co-Optima research and analysis have identified fuel properties that enable advanced boosted SI LD engines
- There are a large number of blendstocks readily derived from biomass (and petroleum) that possess beneficial properties
- Key research needs have been identified for promising blendstock performance, technology, economic, and environmental metrics

Next Steps

- Identify fuel property/engine parameter effects for LD multimode combustion approaches and kinetically controlled combustion
- Complete blendstock survey for advanced diesel (mixing controlled combustion)
- Identify impacts of electrified powertrains on future engine requirements and incorporate into Co-Optima R&D plan

Thank You!

謝謝

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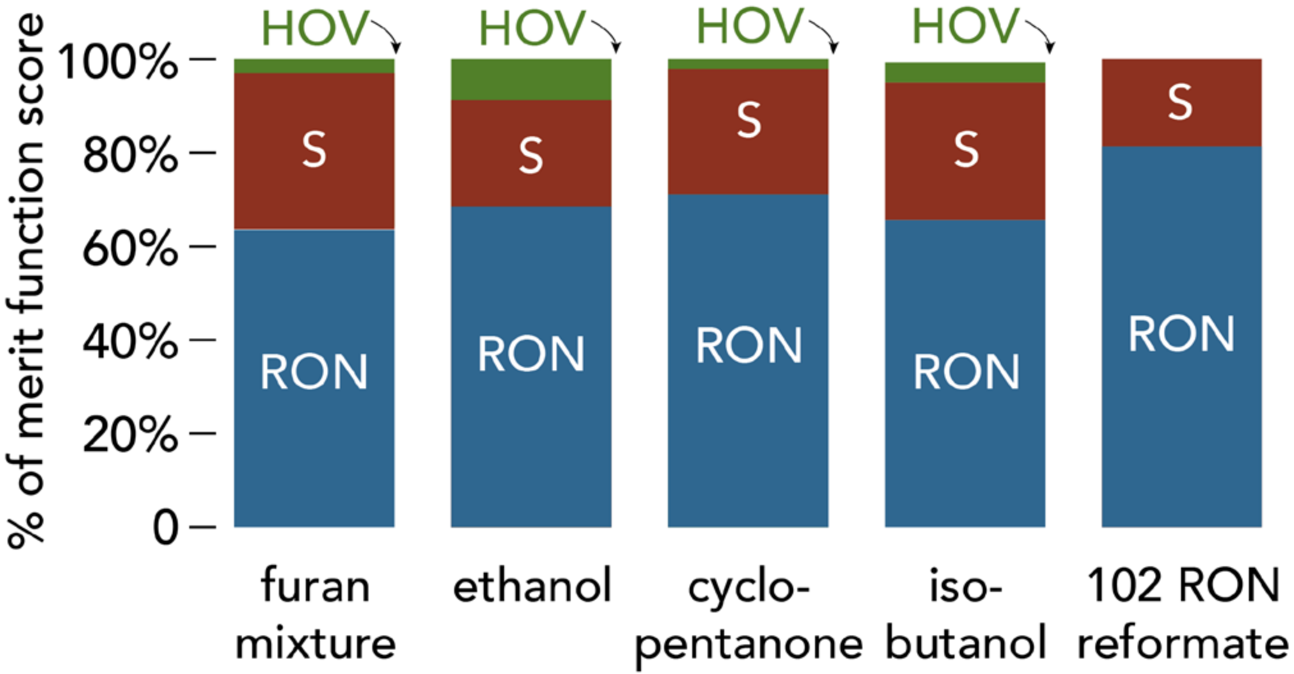
Backup Slides

Relative property benefits differ among blendstocks

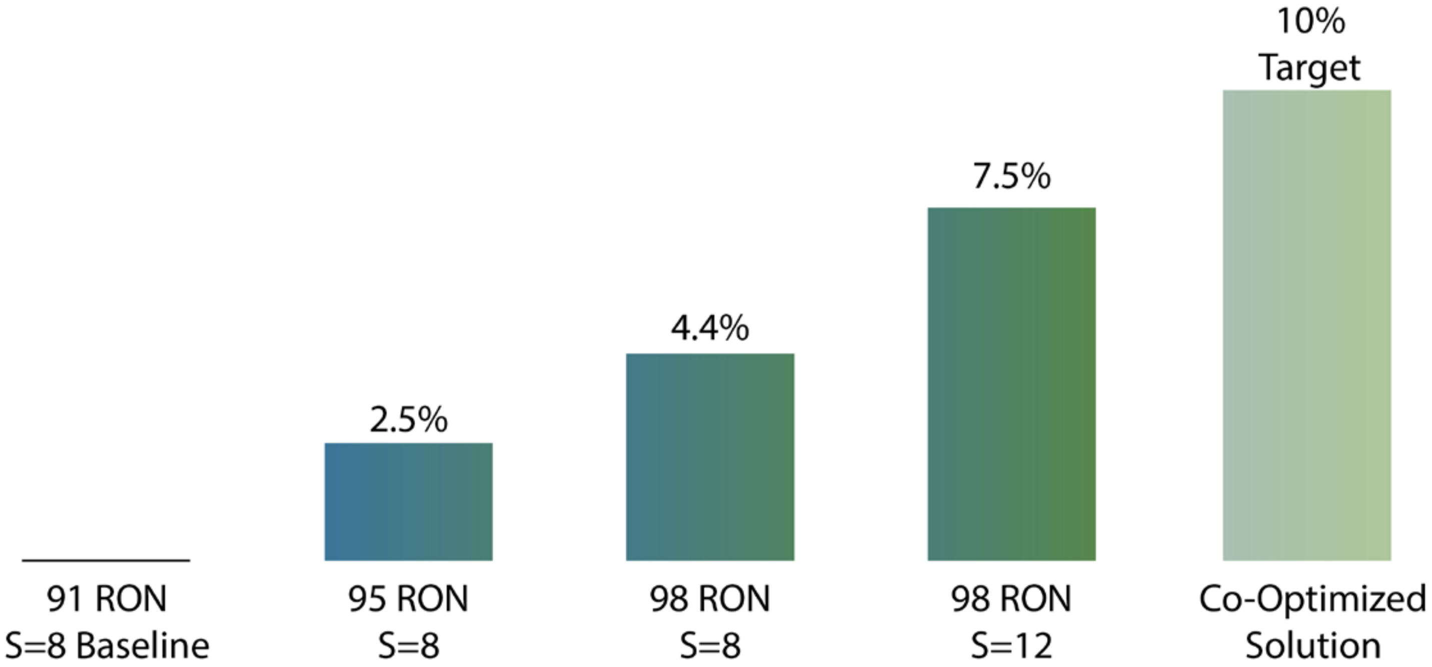


Merit function score correlates fuel properties to engine efficiency relative to U.S. regular gasoline. Data are for 30% blends in a conventional blendstock for oxygenate blending (BOB).*

Average contribution to efficiency merit function for all of the highest scoring blendstocks

* Farrell, John, John Holladay, and Robert Wagner. "Fuel Blendstocks with the Potential to Optimize Future Gasoline Engine Performance: Identification of Five Chemical Families for Detailed Evaluation." Technical Report. U.S. Department of Energy, Washington, DC. 2018. DOE/GO-102018-4970.

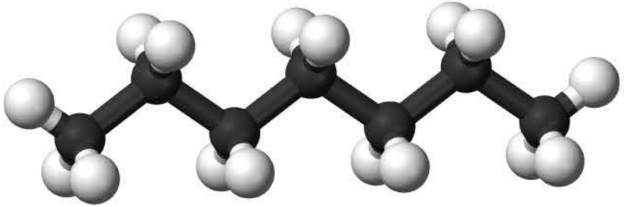
Efficiency Improvement: Boosted SI Engines



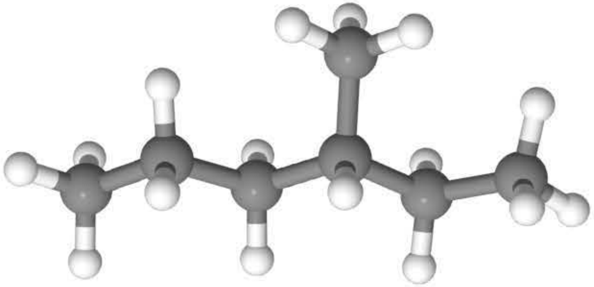
S = sensitivity = RON - MON; Engine efficiencies calculated for conditions appropriate for boosted downsized engines (K = -1.25)

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.

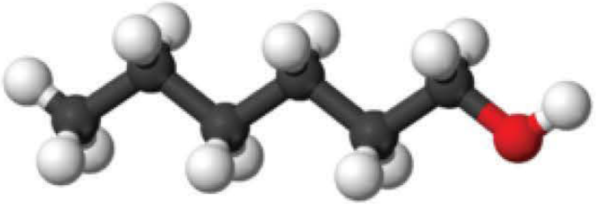
Structure Property Relationships



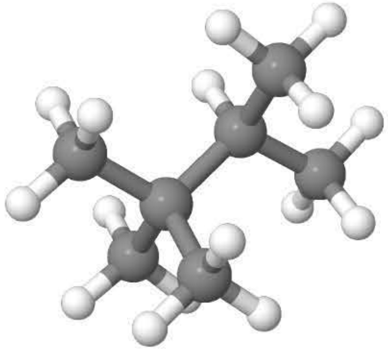
n-heptane (C_7H_{16}): RON = 0, MON=0



3-methylhexane (C_7H_{16}):
RON = 52, MON=56



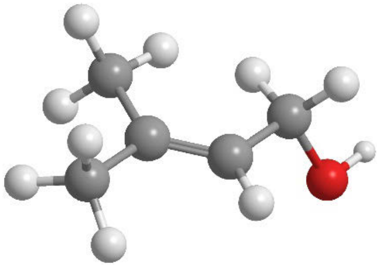
1-hexanol ($C_6H_{13}OH$): RON = 69, MON=64



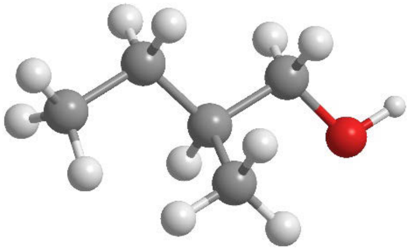
triptane (C_7H_{16}): RON = 112, MON=101

Types and arrangement of atoms impacts properties of blendstocks and guides new blendstock identification

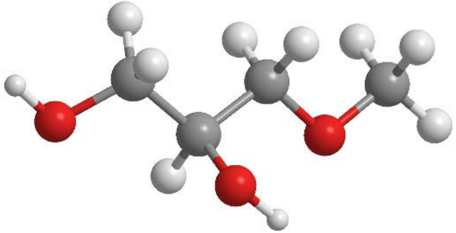
Structure Property Relationships Yield New Blendstocks



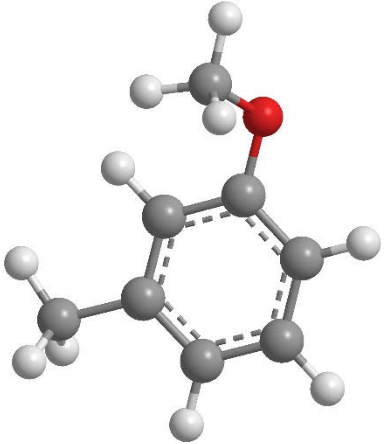
Prenol ($C_5H_{10}O$): RON = 93.5, MON =74



2-Methyl-1-butanol ($C_5H_{12}O$): RON = 102, MON =87.9



Monomethoxyglycerol ($C_4H_{10}O_3$):
DCN = 9.9 (dRON = 100.3)



3-Methylanisole ($C_8H_{10}O$)

Ester Sensitivity Enhanced with Ethanol

- Esters are high-RON, low S blendstocks
- Esters blended into E0 impart no octane sensitivity
- Blending into E10 "turns on" S
- Value proposition:
  - Identify mechanism behind ethanol enhancement
  - Identify bioblendstocks that synergistically blend with ethanol to yield high S