Co-Optimization of Fuels & Engines

better fuels | better vehicles | sooner

An Introduction to DOE's Co-Optima Initiative

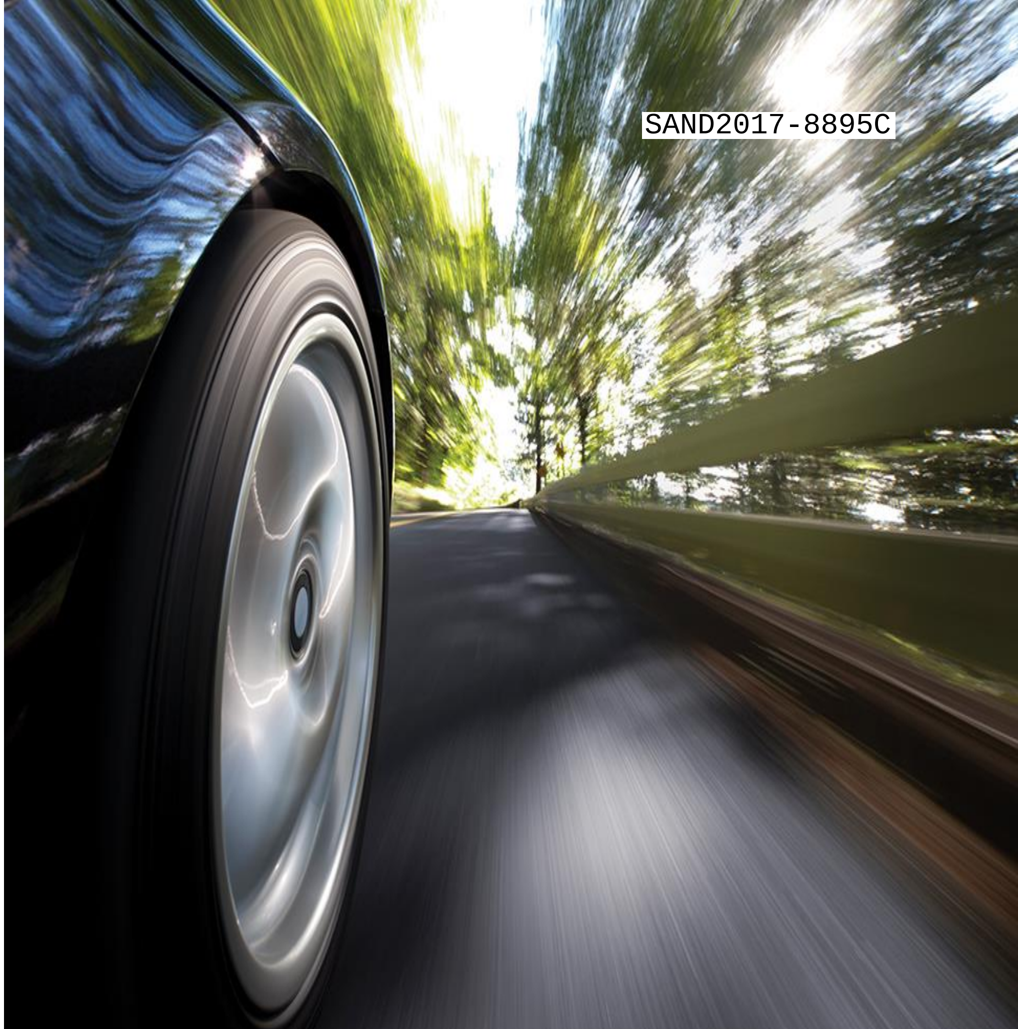
Magnus Sjöberg

Sandia National Laboratories

International Workshop on Fuel & Engine Interactions

August 23, 2017

SAND2017-8895C



Co-Optima Leadership Team:
John Farrell (NREL), John Holladay (PNNL), Chris Moen (SNL), Robert Wagner (ORNL)

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

US Department of Energy (DOE) Bioenergy Technologies Office Program Managers: Alicia Lindauer, Borka Kostova
US DOE Vehicle Technologies Office Program Managers: Gurpreet Singh, Kevin Stork, Leo Breton & Michael Weismiller

Co-Optima Initiative

Started Oct 2016

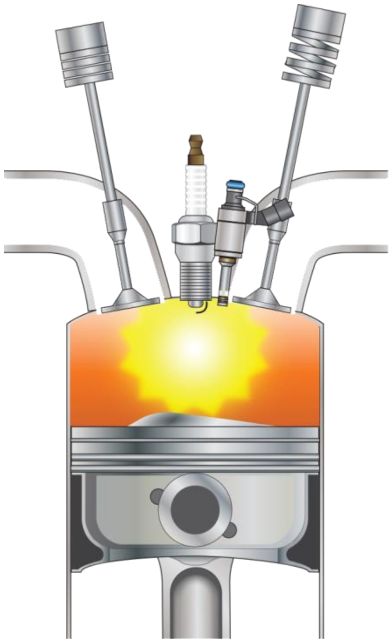
Team:

9 national labs
13 universities

Contributions from numerous researchers acknowledged

Engines: Light, Medium, and Heavy Duty

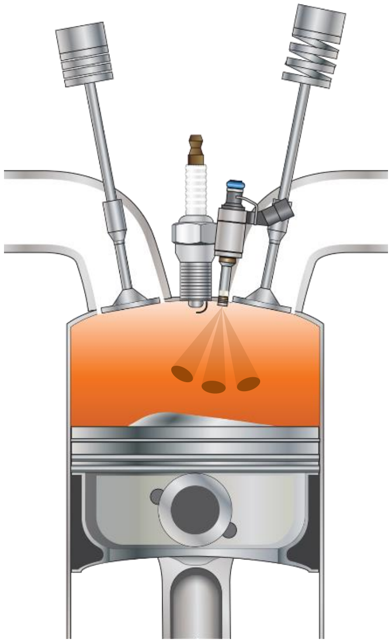
Light-Duty



Boosted SI

Higher efficiency through downsizing

Near-term

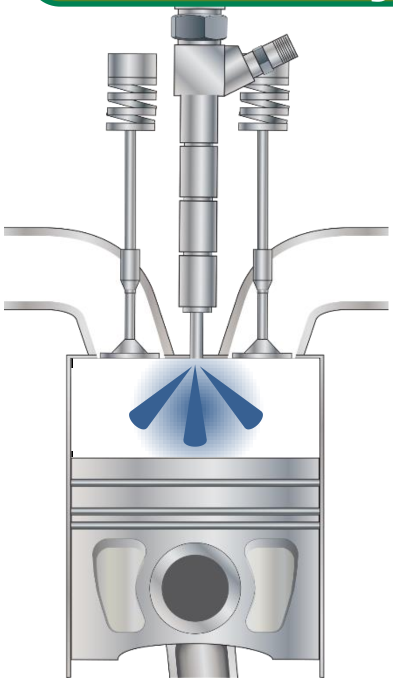


Multi-mode SI / ACI

Even higher efficiency over drive cycle

Mid-term

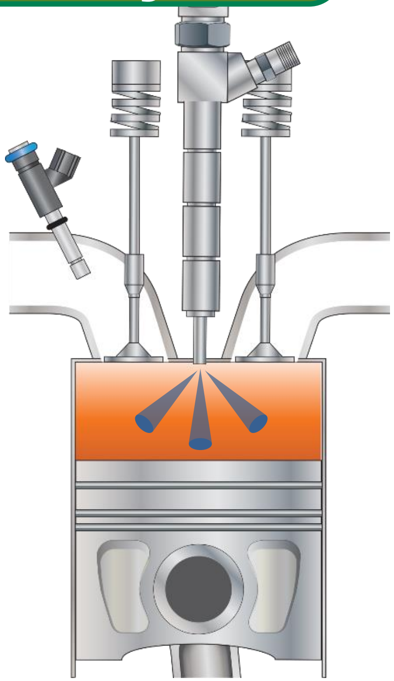
Medium and Heavy-Duty



Mixing Controlled

Improved engine emissions

Near-term



Kinetically Controlled

Highest efficiency and emissions performance

Longer-term

Governing Hypotheses

Central Engine Hypothesis

There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

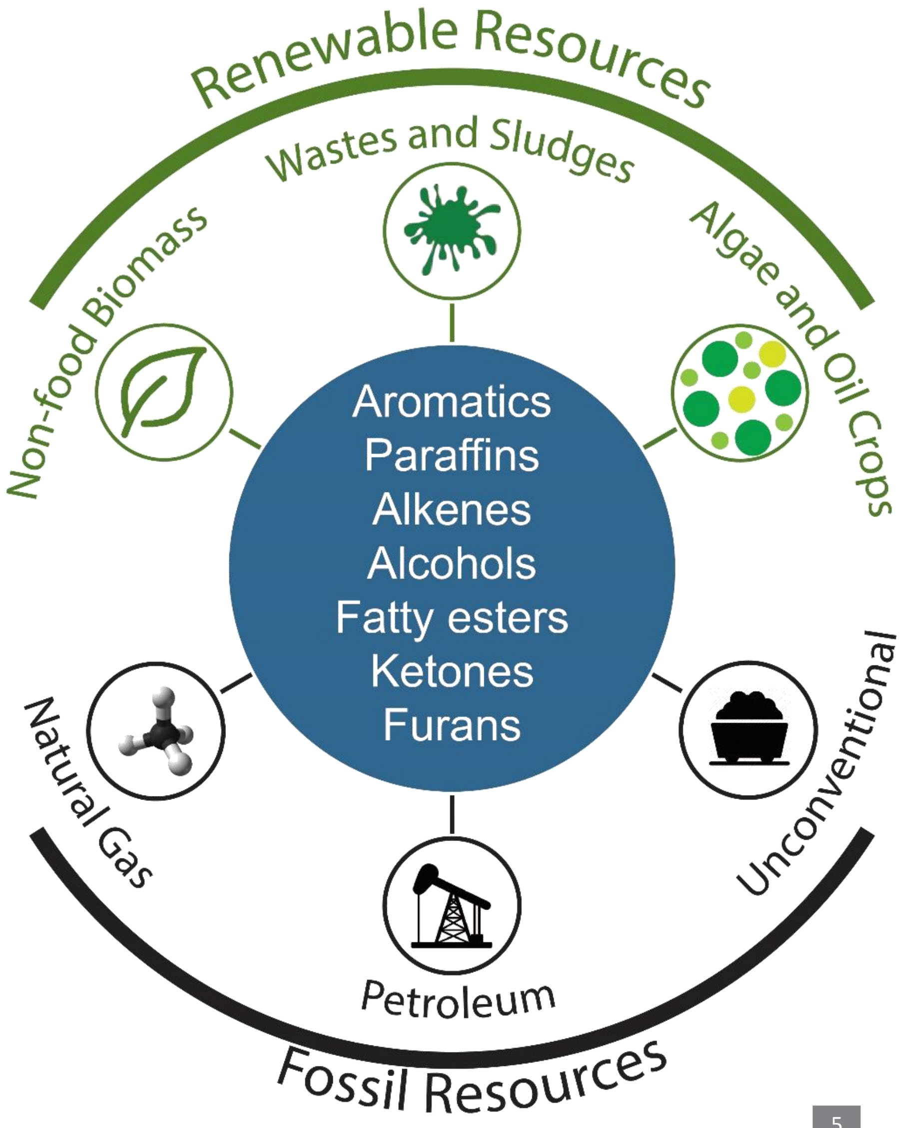
Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance

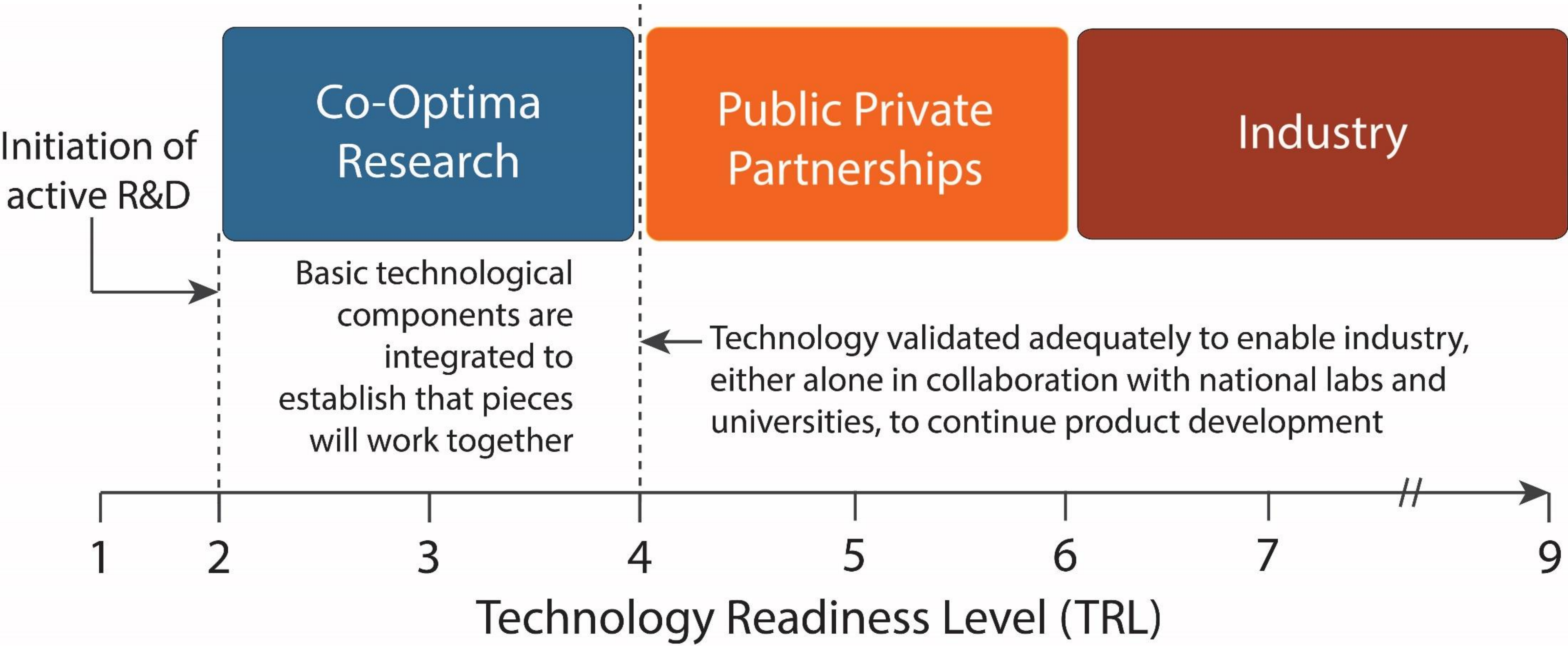
Approach: Fuel-Property Based, Composition-Agnostic

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



Integration with Industry



See https://en.wikipedia.org/wiki/Technology_readiness_level

Introducing New Fuels and Engines Impacts a Large Body of Stakeholders

Energy Companies

Refiners

Biofuel Producers

Fuel Distribution

Government/
Regulatory Agencies

LD OEMs

HD OEMs

Retail

Consumer

Society

Understanding stakeholder value propositions is essential to Co-Optima

Achieving a win-win-win means (ideally) that all stakeholders make money

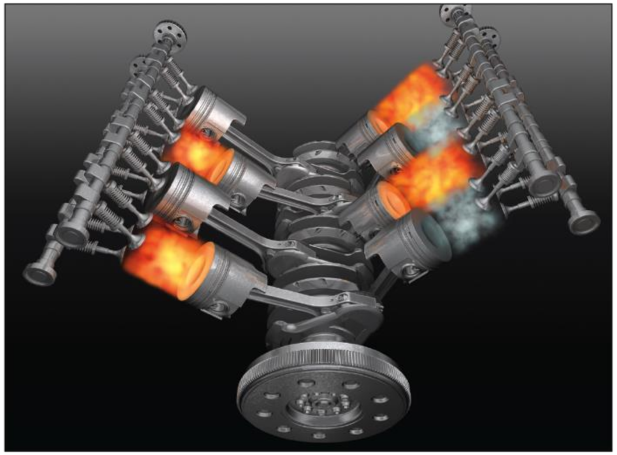
From a research perspective, this means that we're working on the right problems

Co-Optima Technical Challenges

What fuels do engines *really* want?

What fuels *should* we make?

What will work in the real world?



What Fuel Do SI Engines Really Want? More Than Octane

$$\text{Merit} = \alpha \bullet f(RON) + \beta \bullet f(K, S) + \gamma \bullet f(HOV) + \varepsilon \bullet f(S_L) + \zeta \bullet f(PMI) + \eta \bullet f(T_{c,90,conv})$$

- RON: $\alpha \bullet f(RON)$
- Octane Sensitivity: $\beta \bullet f(K, S)$
- Heat of Vaporization: $\gamma \bullet f(HOV)$
- Flame Speed: $\varepsilon \bullet f(S_L)$
- PM Emissions: $\zeta \bullet f(PMI)$
- Catalyst Light-off Temp (cold start): $\eta \bullet f(T_{c,90,conv})$

• Merit function quantifies impact of fuel properties on engine efficiency

* Sensitivity = RON – MON; HOV = heat of vaporization

What Fuel Do SI Engines Really Want? More Than Octane

Octane Index: RON, Octane Sensitivity

Charge Cooling: Heat of Vaporization

$$\text{Merit} = \alpha \bullet f(\text{RON}) + \beta \bullet f(K, S) + \gamma \bullet f(\text{HOV}) + \varepsilon \bullet f(S_L) + \zeta \bullet f(\text{PMI}) + \eta \bullet f(T_{c,90,conv})$$

RON: $\alpha \bullet f(\text{RON})$

Octane Sensitivity: $\beta \bullet f(K, S)$

Heat of Vaporization: $\gamma \bullet f(\text{HOV})$

Flame Speed: $\varepsilon \bullet f(S_L)$

PM Emissions: $\zeta \bullet f(\text{PMI})$

Catalyst Light-off Temp (cold start): $\eta \bullet f(T_{c,90,conv})$

Dilution Tolerance: Flame Speed

Emissions Penalties: PM Emissions, Catalyst Light-off Temp (cold start)

- Merit function quantifies impact of fuel properties on engine efficiency

* Sensitivity = RON – MON; HOV = heat of vaporization

Octane Index Framework

Beyond MON | **MON** | **RON** | **Beyond RON**

K > 1
Ex: Heated intake / high residuals HCCI

Higher Temperature for a given Pressure
K=1

Lower Temperature for a given Pressure
K=0

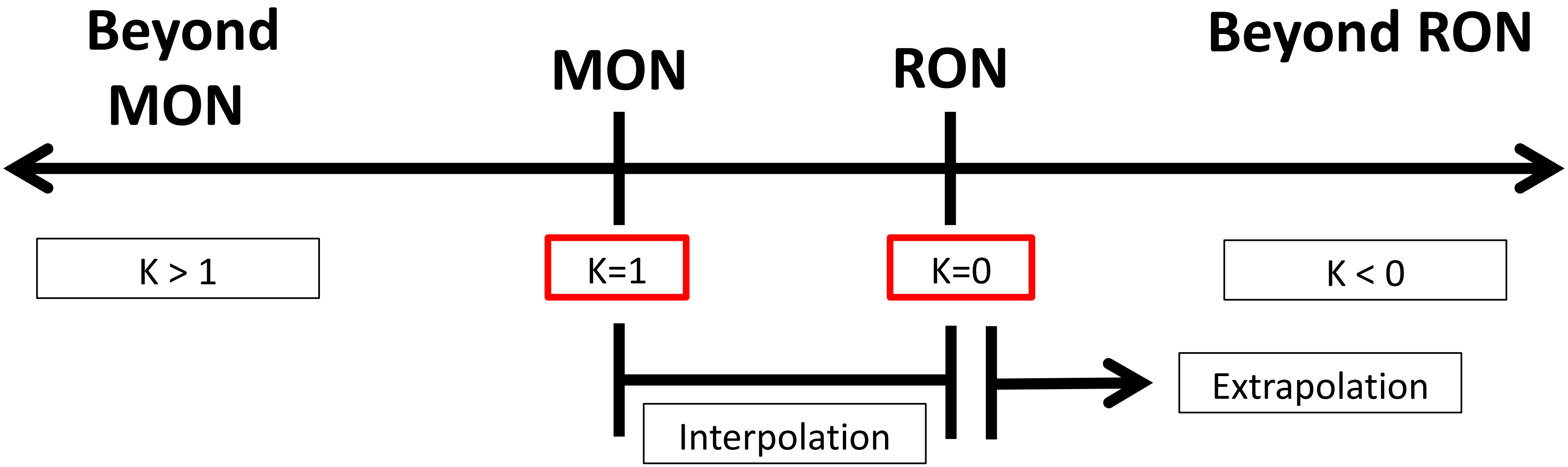
K < 0
Ex: Boosted SI, GCI

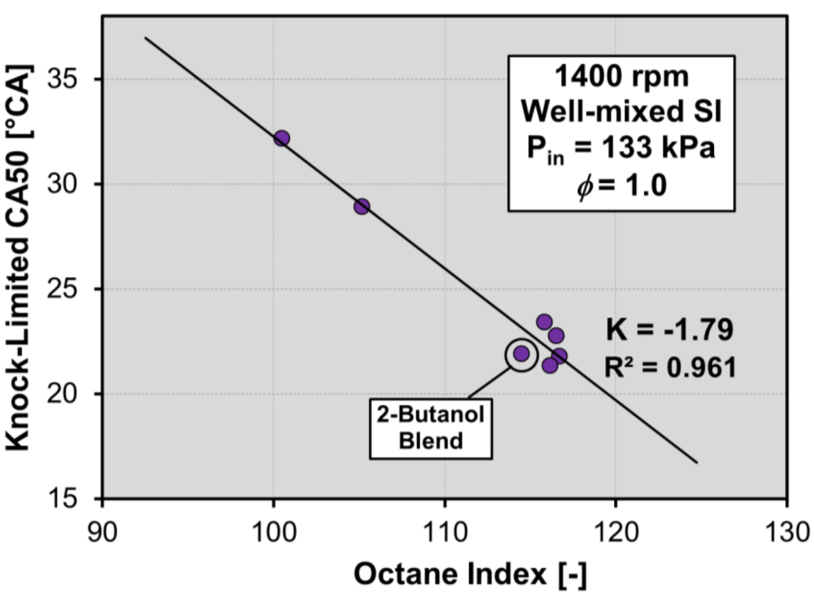
Octane Index = RON – K • S

S = RON - MON

K = Determined by operating condition

Octane Index Framework



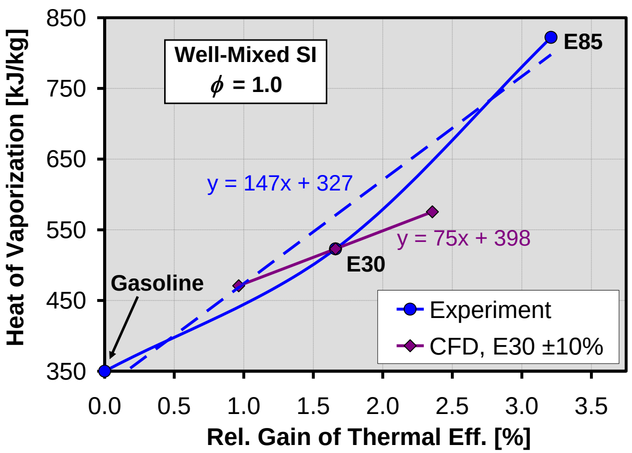


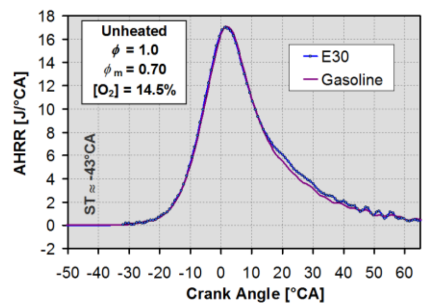
Modern SI Engines

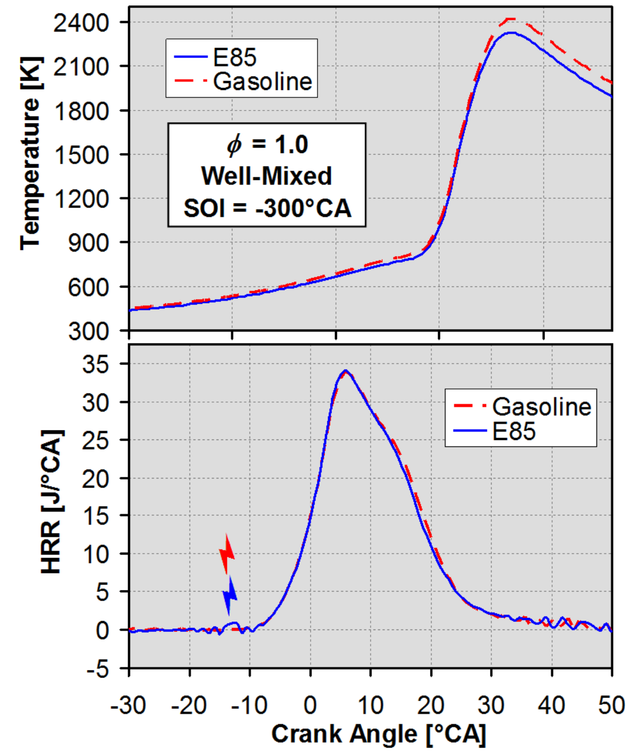
- 2-Butanol blend outperforms OI prediction.
- Moderate challenge to Central Fuels Hypothesis.

Merit Function Development
HoV Benefit

- Gasoline-ethanol blends are uniquely qualified for assessing direct gain of higher HoV on η_{th} for non-knock limited SI operation.
  - Inherent higher flame speed of ethanol compensates perfectly for lower charge temp. with higher HoV.
  - Examples for stoichiometric dilute and non-dilute operation.







- Available data support HoV benefits of originally proposed Merit Function.

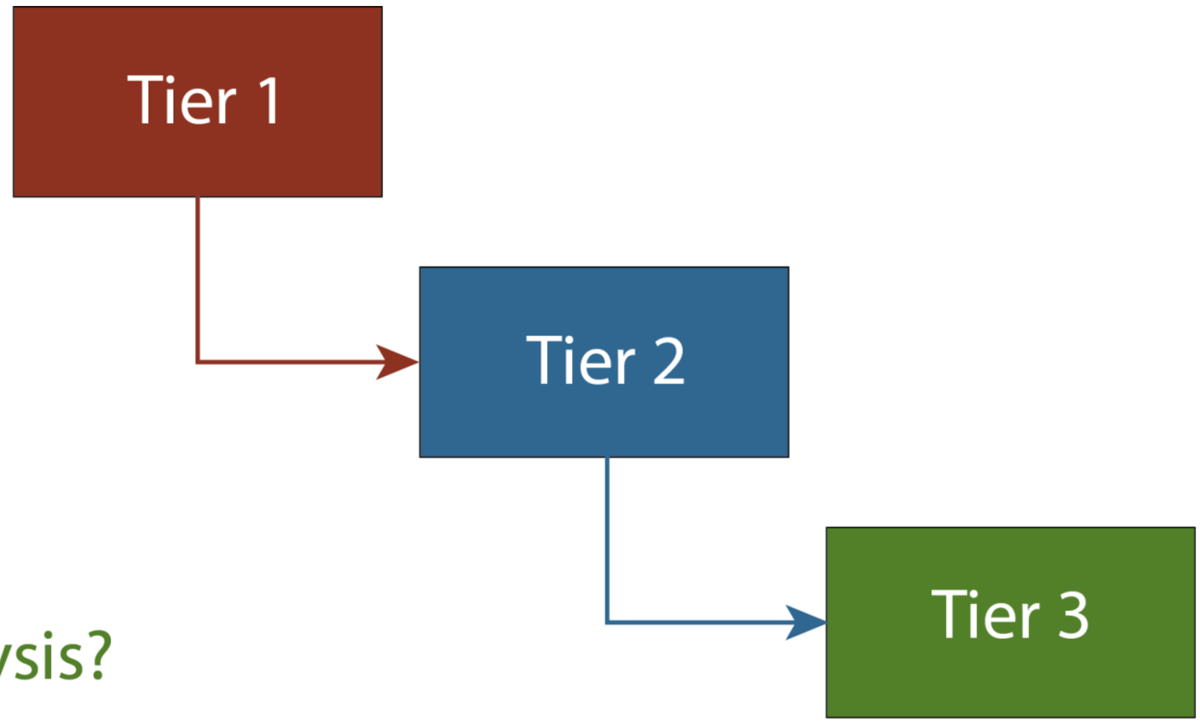
- CFD results indicate that incremental benefit per [kJ/kg] of HoV is higher than what is realized across full E0 – E85 range.
  - Justifies further examination.

What Fuels Should We Make?
Comprehensive Blendstock Survey Completed

Can it be a fuel?

Does it provide desired performance?

Does it merit focused experiments and analysis?



blendstocks: > 400 | ~ 40 | < 10

Tiered Blendstock Identification

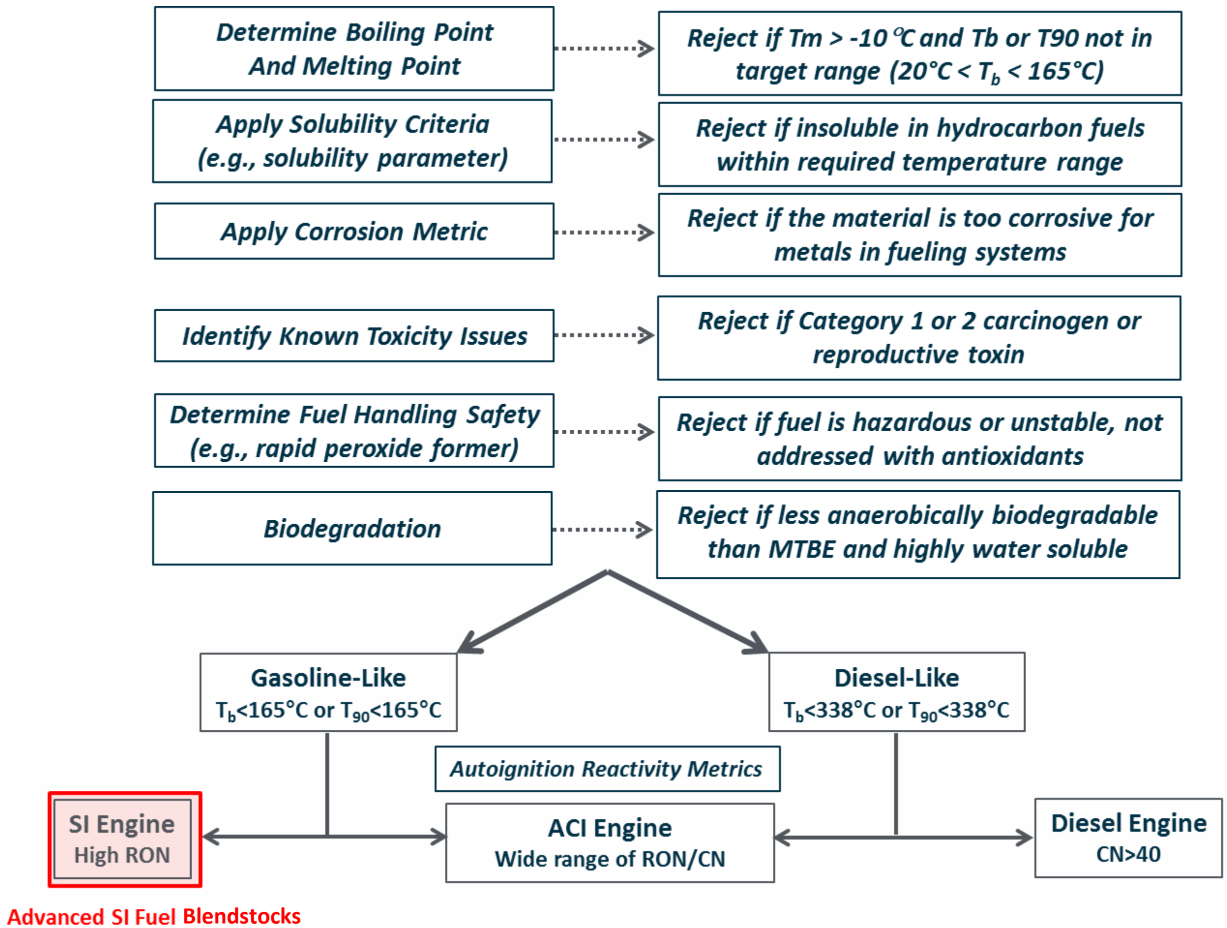
Tier 1

> 470 blendstocks

14 chemical families

Identify broad range of potential hydrocarbon and oxygenated blendstocks

Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks



Boosted SI Tier 2 blendstocks

	Alcohols (9)
1	Methanol
2	Ethanol
3	1-Propanol
4	Isopropanol
5	1-Butanol
6	2-Butanol
7	Isobutanol
8	2-Methylbutan-1-ol
9	2-Pentanol

	Ethers
10	Anisole

	Esters (13)
11	Methyl acetate
12	Methyl butanoate
13	Methyl pentanoate
14	Methyl isobutanoate
15	Methyl-2-methylbutanoate

	Esters (13)
16	Ethyl acetate
17	Ethyl butanoate
18	Ethyl isobutanoate
19	Isopropyl acetate
20	Butyl acetate
21	2-Methylpropyl acetate
22	3-Methylpropyl acetate
23	mixed esters

	Ketones (9)
24	2-Butanone
25	2-Pentanone
26	3-Pentanone
27	Cyclopentanone
28	3-Hexanone
29	4-Methyl-2-Pentanone
30	2,4-Dimethyl-3-Pentanone
31	3-Methyl-2-butanone
32	Ketone mixture

	Furans
33	2,5-Dimethylfuran/2-methylfuran

	Branched alkanes
34	2,2,3-Trimethylbutane

	Alkenes
35	Diisobutylene

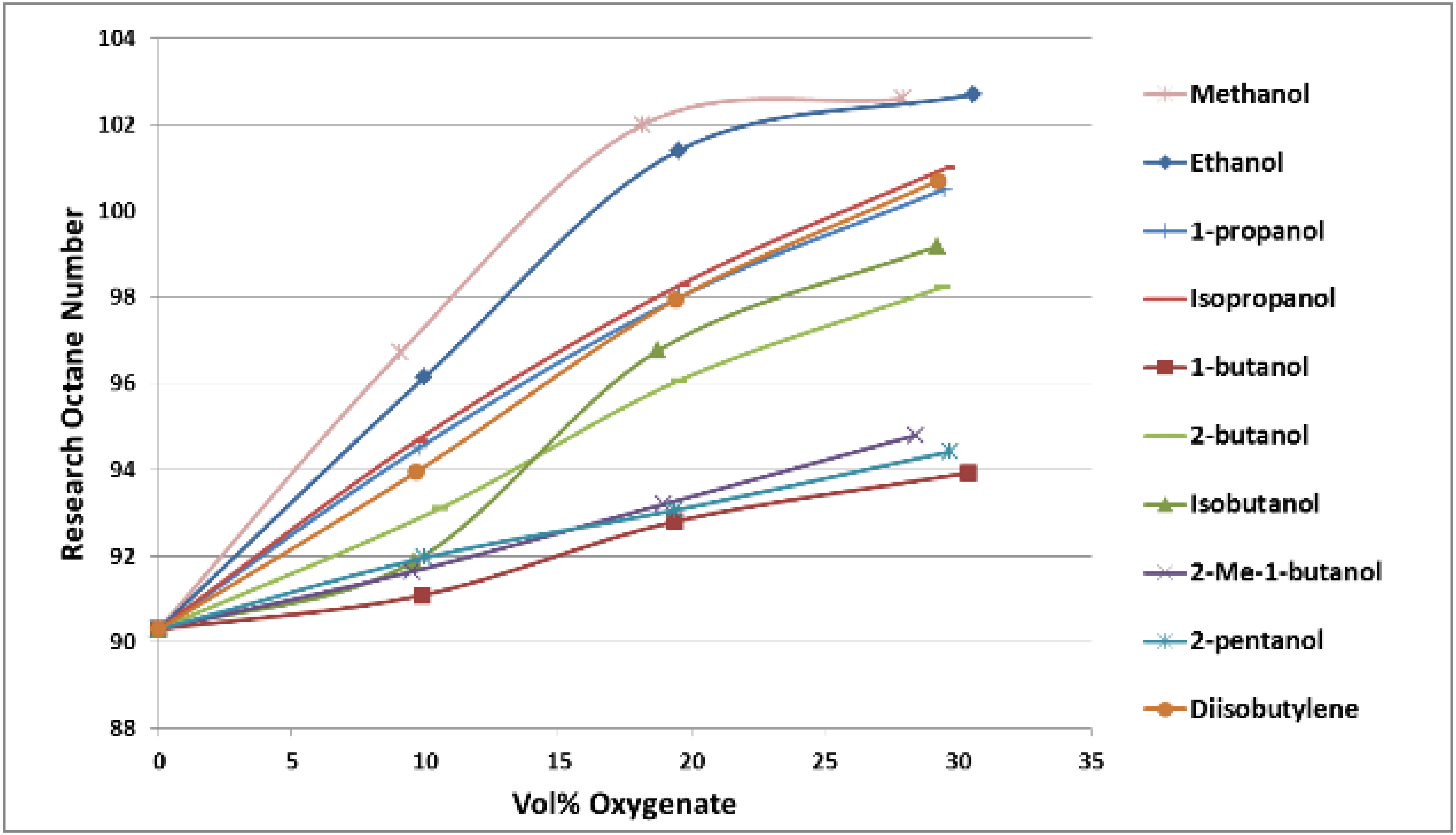
	Multicomponent mixtures (6)
36	Methanol-to-gasoline
37	Ethanol-to-gasoline
38	Bioreformate via multistage pyrolysis
39	Bioreformate via catalytic conversion of sugar
40	Mixed aromatics via catalytic fast pyrolysis
41	Aromatics and olefins via pyrolysis-derived sugars

Merit Function

$$Merit = \frac{(RON_{mix} - 91)}{1.6} - K\frac{(S_{mix} - 8)}{1.6}$$
$$+ \frac{0.085[ON / kJ / kg_{mix}] \cdot ((HoV_{fuel} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1)))}{1.6}$$
$$+ \frac{((HoV_{mix} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1)))}{15.2} + \frac{(S_{L,mix} - 46[cm / s])}{5.4}$$
$$- H(PMI_{mix} - 1.6)[0.7 + 0.5(PMI_{mix} - 1.4)] + 0.008\,°C^{-1}\left(T_{c,90,conv} - T_{c,90,mix}\right)$$

- Major changes (March 2017 revision):
  - Updated coefficients for RON, S, HoV, S_L, and PMI
  - Deletion of term for low-speed pre-ignition (LSPI)
  - Addition of term to reflect cold start

Blending Octane Data



Merit Function Scores – modeled (K = - 1.25)

	10%			20%			30%			10%			20%			30%				
Blendstock	cBOB	CARBOB	sBOB	cBOB	CARBOB	sBOB	cBOB	CARBOB	sBOB	F1 BOB	F2 BOB	F3 BOB	F1 BOB	F2 BOB	F3 BOB	F1 BOB	F2 BOB	F3 BOB	Green	Yellow
Furan Mixture	8.6	1.9	5.1	12.8	6.8	9.6	12.9	7.7	10.2	1.1	5.1	9.0	6.1	9.6	13.1	7.1	10.2	13.2	14	2
Methanol	7.1	0.3	3.6	15.0	9.0	11.9	15.6	10.4	12.9	(0.4)	3.5	7.4	8.4	11.9	15.3	9.8	12.9	15.9	14	0
Ethanol	5.7	(1.1)	2.2	12.2	6.2	9.1	12.7	7.5	10.0	(1.8)	2.1	6.0	5.6	9.1	12.5	6.9	10.0	13.0	13	1
n-propanol	4.4	(2.3)	0.9	8.5	2.6	5.4	11.6	6.4	8.9	(3.0)	0.9	4.8	1.9	5.4	8.8	5.8	8.9	11.9	8	3
Diisobutylene	2.9	(3.8)	(0.6)	7.7	1.7	4.5	11.0	5.7	8.3	(4.5)	(0.6)	3.3	1.0	4.5	8.0	5.2	8.2	11.2	7	1
Isobutanol	1.0	(5.8)	(2.6)	7.3	1.3	4.2	10.2	4.9	7.4	(6.5)	(2.6)	1.3	0.6	4.1	7.6	4.4	7.4	10.4	6	1
Cyclopentanone	2.8	(3.9)	(0.7)	6.5	0.6	3.4	10.4	5.1	7.6	(4.6)	(0.7)	3.2	(0.1)	3.4	6.8	4.6	7.6	10.6	6	1
iso-propanol	4.0	(2.7)	0.5	7.2	1.2	4.1	9.8	4.6	7.1	(3.4)	0.5	4.4	0.6	4.1	7.5	4.0	7.1	10.1	6	0
2-butanol	2.2	(4.5)	(1.3)	5.4	(0.5)	2.3	7.5	2.3	4.8	(5.2)	(1.3)	2.6	(1.2)	2.3	5.7	1.7	4.8	7.8	3	3
Anisole	1.9	(4.8)	(2.6)	4.8	(1.2)	1.7	7.9	2.7	5.2	(5.6)	(1.6)	2.2	(1.8)	1.7	5.1	2.1	5.2	8.2	2	4
2-butanone (MEK)	1.1	(5.6)	(2.4)	4.0	(2.0)	0.9	6.0	0.8	3.3	(6.4)	(2.4)	1.4	(2.6)	0.9	4.3	0.2	3.3	6.3	2	0
Methyl acetate	0.8	(5.9)	(2.7)	3.7	(2.3)	0.6	6.2	1.0	3.5	(6.7)	(2.7)	1.1	(2.9)	0.6	4.0	0.4	3.5	6.5	2	0
Ethyl butanoate	0.8	(5.9)	(2.7)	2.7	(3.3)	(0.5)	5.5	0.2	2.8	(6.6)	(2.7)	1.2	(4.0)	(0.5)	3.0	(0.3)	2.7	5.8	1	1
2-Me-1-butanol	1.1	(5.6)	(2.4)	3.3	(2.7)	0.2	5.2	(0.1)	2.5	(6.3)	(2.4)	1.5	(3.4)	0.1	3.6	(0.6)	2.4	5.4	0	2
Ethyl acetate	0.5	(6.3)	(3.0)	2.9	(3.1)	(0.2)	4.9	(0.4)	2.1	(7.0)	(3.1)	0.8	(3.7)	(0.2)	3.2	(1.0)	2.1	5.1	0	2
1-butanol	(0.1)	(6.9)	(3.6)	3.4	(2.6)	0.3	4.6	(0.7)	1.9	(7.6)	(3.7)	0.2	(3.2)	0.3	3.7	(1.2)	1.8	4.8	0	1
3-Me-1-butanol	(0.0)	(6.7)	(3.5)	1.4	(4.6)	(1.7)	2.9	(2.4)	0.2	(7.5)	(3.5)	0.3	(5.2)	(1.7)	1.7	(2.9)	0.1	3.2	0	0
Butyl acetate	(0.2)	(6.9)	(3.7)	0.9	(5.1)	(2.2)	1.1	(4.2)	(1.6)	(7.7)	(3.7)	0.1	(5.7)	(2.2)	1.2	(4.7)	(1.7)	1.3	0	0
2,4 dimethyl-3- pentanone	(2.3)	(9.0)	(5.8)	(0.3)	(6.3)	(3.4)	0.7	(4.5)	(2.0)	(9.7)	(5.8)	(1.9)	(7.0)	(3.5)	(0.0)	(5.1)	(2.1)	1.0	0	0
2-pentanone	1.2	(5.5)	(2.3)	2.8	(3.1)	(0.3)	3.4	(1.8)	0.7	(6.2)	(2.3)	1.6	(3.8)	(0.3)	3.1	(2.4)	0.6	3.7	0	0
2-pentanol	1.3	(5.5)	(2.2)	1.9	(4.1)	(1.3)	3.1	(2.1)	0.4	(6.2)	(2.3)	1.6	(4.8)	(1.3)	2.2	(2.7)	0.4	3.4	0	0
Ketone Mixture	(0.9)	(7.6)	(4.4)	(1.2)	(7.2)	(4.4)	(0.7)	(6.0)	(3.4)	(8.3)	(4.4)	(0.5)	(7.9)	(4.4)	(0.9)	(6.5)	(3.5)	(0.5)	0	0
Triptane	(0.2)	(6.9)	(3.7)	(0.3)	(6.3)	(3.4)	2.1	(3.2)	(0.7)	(7.7)	(3.7)	0.2	(6.9)	(3.4)	0.0	(3.8)	(0.7)	2.3	0	0

cBOB: conventional blendstock for oxygenated blending (premium)

CARBOB: California Reformulated Gasoline BOB

sBOB: Summer BOB

F1 BOB: 86 RON (S = 2)

F2 BOB: 86 RON (S = 8)

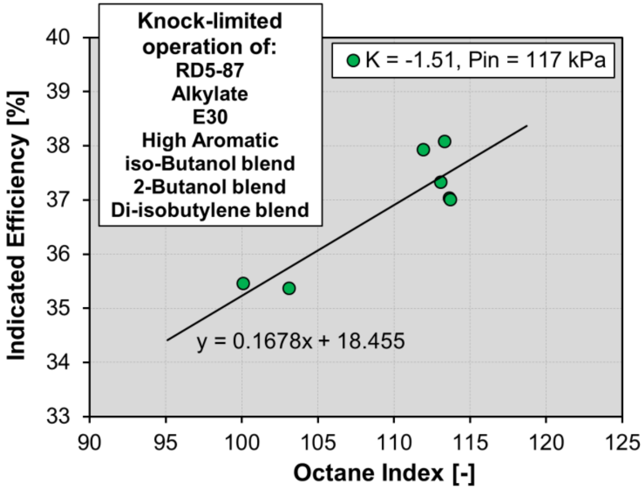
F3 BOB: 86 RON (S = 13)

Deeper look at merit function scores

cBOB 30% blending

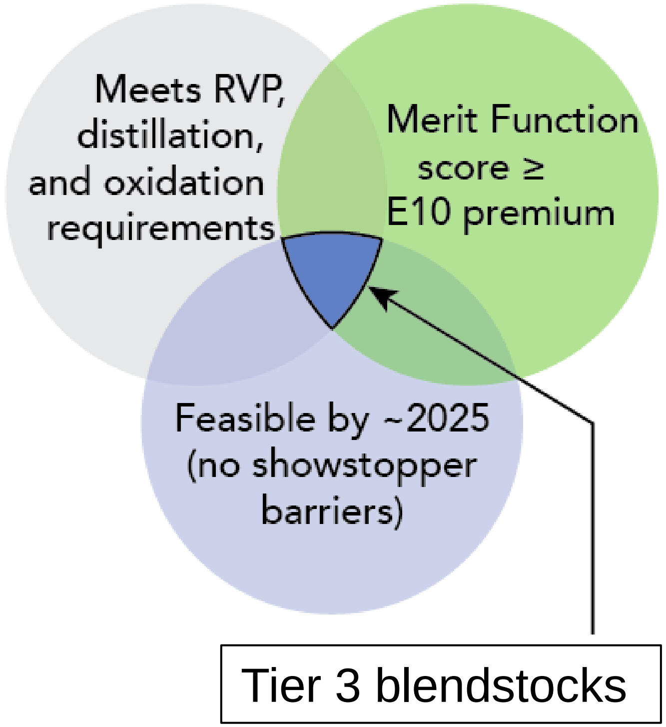
Blendstock	Total Merit	RON	S	HoV	(RON+S)/MF
Methanol	15.6	9.3	4.1	2.25	0.86
Furan Mixture	12.9	8.2	4.3	0.39	0.97
Ethanol	12.7	8.7	2.9	1.24	0.90
Diisobutylene	11.0	7.7	4.0	-0.73	1.1
Cyclopentanone	10.4	7.4	2.8	0.08	0.99
Isobutanol	10.2	6.7	3.0	0.43	0.96

- RON and S contributions dominate merit function scores.
- BOB properties (e.g., S) can significantly impact scores.
- Need to account for uncertainty, both in merit function properties (RON, etc) as well as merit function itself.
- Need to explore impact of K



Tier 2 to Tier 3 transition criteria

1. Meet current critical fuel specs (RVP, distillation, oxidative stability, etc.) when blended in petroleum BOB*
2. Achieve merit function score ≥ E10 premium when blended in petroleum BOB*
3. No “showstopper” barriers
   - Blendstocks must have viable path to potential market introduction by ~2025-2030



Tier 2 → 3 transition allows focused effort on blendstocks with greatest potential to meet Co-Optima goals

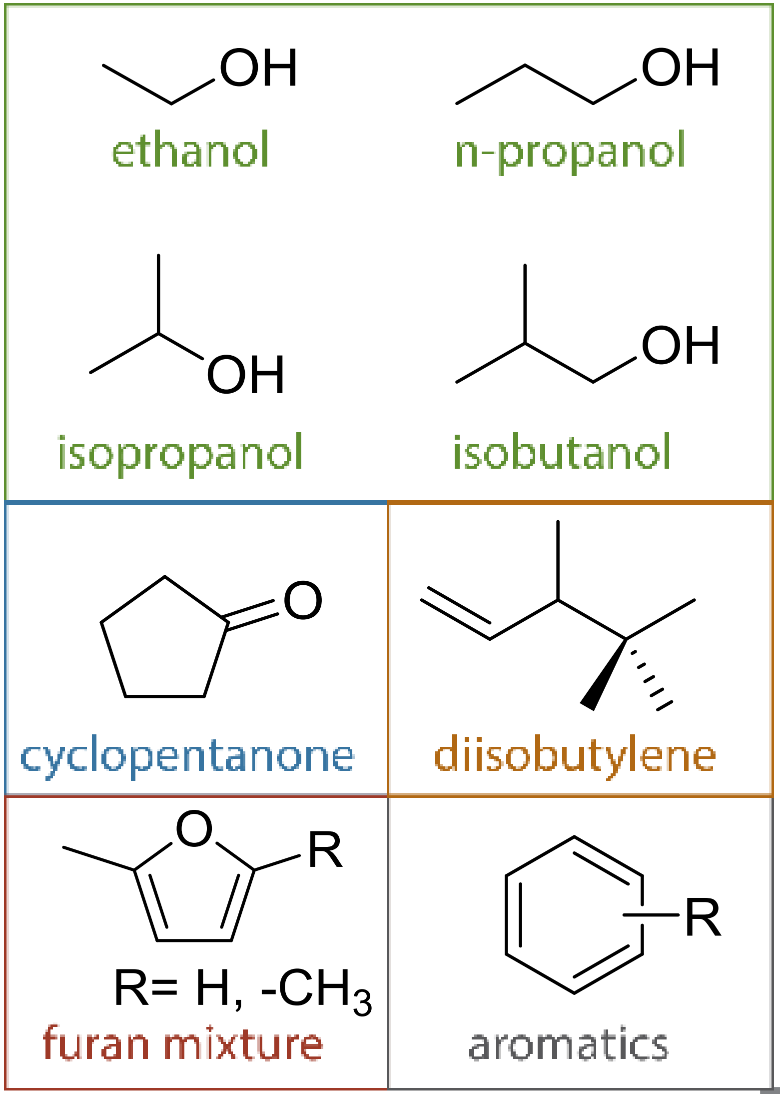
* Evaluated at blend levels of 10, 20, and 30% by volume

High performing boosted SI blendstocks identified

Properties provided by chemical families:

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

Representative Tier 3 blendstocks



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

What Will Work in the Real World?

Blendstocks with feasible pathways to large scale production by ~2025-2030 identified via integrated systems-level analyses

Technology Readiness

- State of technology: Fuel production
- 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

Market

- Uncertainty
- Regulatory requirements
- Geographic factors
- Political factors
- Vehicle compatibility
- Infrastructure compatibility

↑ Assessed only for blendstocks produced from biomass (Technology Readiness, Environmental, Economics)

↑ Independent of blendstocks source (Market)

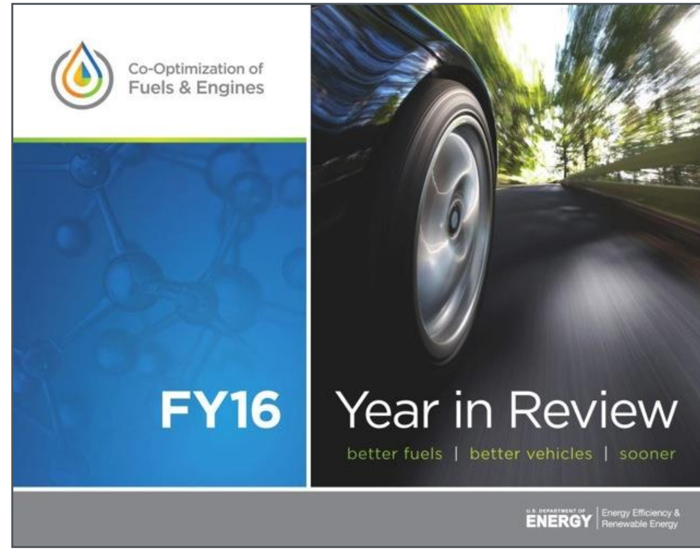
Documenting Key Findings for Stakeholders

Reports highlighting Co-Optima accomplishments:

- FY16 Year in Review
- Fuel Blendstocks with the Potential to Optimize Boosted Spark-Ignition Engine Performance§

Reports being published examine issues relevant to new fuel/vehicle introductions:

- Fuel and vehicle introduction§
- Fuel and vehicle distribution§
- Lessons learned from first generation ethanol§
- Misfueling mitigation*



* http://www.nrel.gov/docs/fy17osti/66918.pdf

§ in press

Co-Optima Research Setting the Foundation for Creating a Win-Win-Win for Stakeholders

- Research guided by value propositions for all stakeholders key to accelerating introduction of new fuels and vehicles
- Co-Optima research is providing the data, tools, and knowledge to inform stakeholders and decision makers
- Fuel property focus and technology neutral approach allows for market-driven, industry-led solutions

Acknowledgement

- The experimental work related to the octane-index framework and heat of vaporization presented here was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA.
- Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.