Co-Optimization of Fuels & Engines

Co-Optimization of Fuels & Engines (Co-Optima) Initiative

John Farrell, National Renewable Energy Lab

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

Acknowledgments

DOE Sponsors:

Alicia Lindauer and Borka Kostova (BETO)

Kevin Stork, Gurpreet Singh, Leo Breton, and Mike Weismiller (VTO)

Co-Optima Technical Team Leads:

Dan Gaspar (PNNL), Paul Miles (SNL), Jim Szybist (ORNL),

Jennifer Dunn (ANL), Matt McNenly (LLNL), Doug Longman (ANL)

Other Co-Optima Leadership Team Members:

John Holladay (PNNL), Robert Wagner (ORNL), Chris Moen (SNL)

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?

Governing Hypotheses

Central Engine Hypothesis

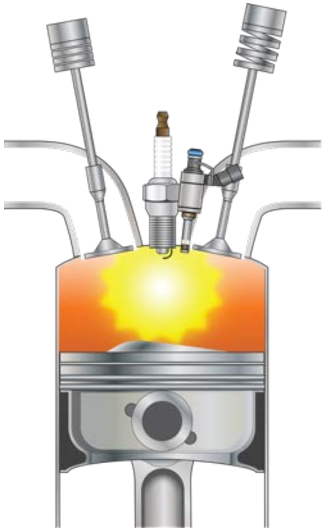
There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

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

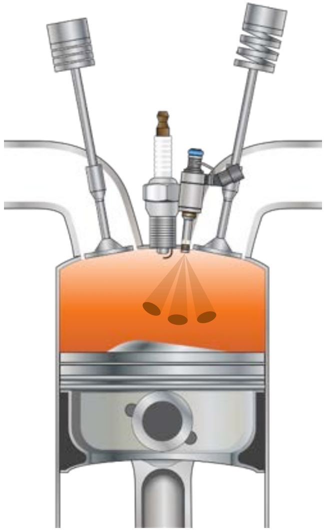
Two Parallel R&D Projects

Light-Duty



Boosted SI

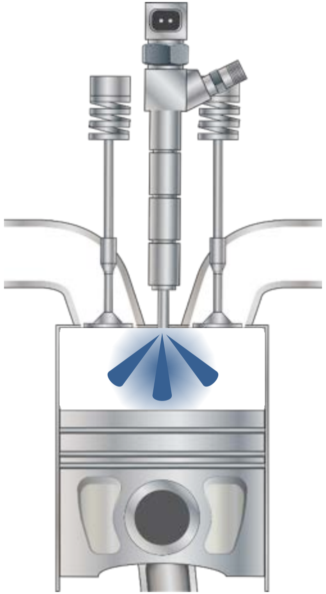
Near-term



Multi-mode SI/ACI

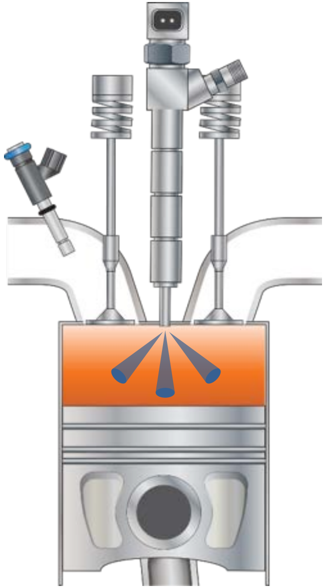
Mid-term

Medium/Heavy-Duty



Mixing Controlled

Near-term



Kinetically Controlled

Longer-term

High-level goals and outcomes

Light-duty

Up to 15% fuel economy (FE) improvement* 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. The team is actively engaging with OEMs, fuel providers, and other key stakeholders to refine goals and approaches to measuring fuel economy improvements

Co-Optima Team

Nine national labs,
13 universities

> 100 researchers,
> 75 projects

External Advisory Board

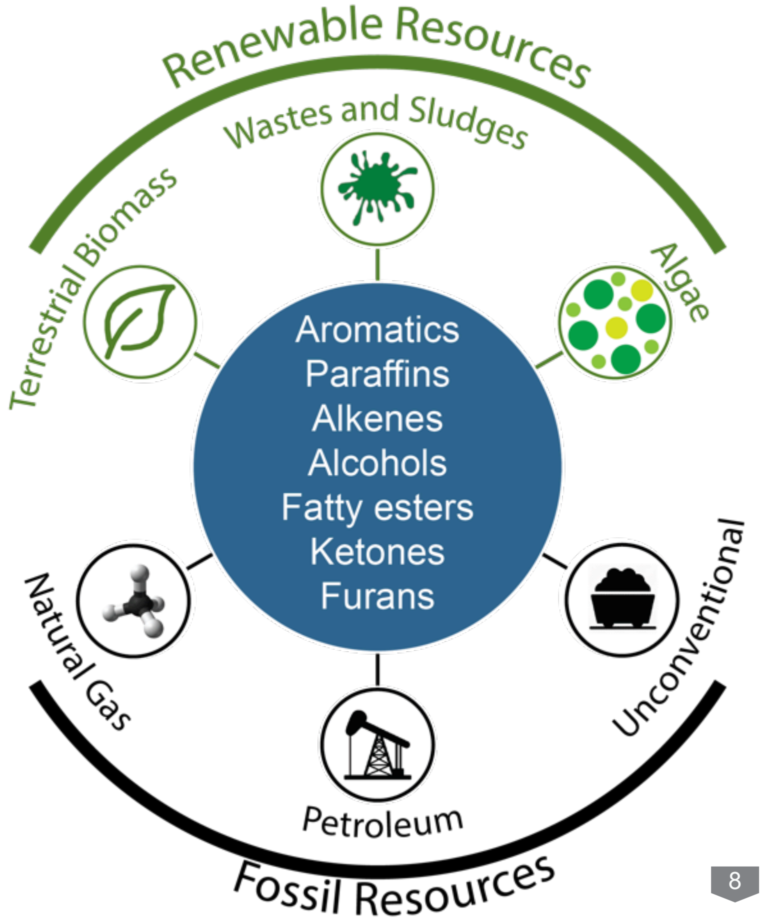
77 stakeholder organizations

Budget: FY16: $26M
FY17: $24.5

Approach

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

* We are not going to recommend that <u>any</u> specific blendstocks be included in future fuels



Systematic Blendstock Survey

Objective: identify a broad range of feasible blendstock options

Primary focus: identify blendstocks with desired properties that have a strong potential to be sourced from biomass

Potential Benefits of Biomass Sourced Fuel

Technical

Tailor fuel properties desired in the blendstock

Add value to refiners – blend up low quality (inexpensive) petroleum blendstocks

Help refiners balance global trends in transportation fuel use

Societal

Reliable domestic energy options that are affordable & efficient

Strengthens energy security by increasing supply, diversity, reliability

Retain $260 billion in the U.S.

Add 1.1M direct jobs

Expand U.S. science/ technology leadership

Environmental

Reduce emissions, including CO_2 emissions, by 450 million tons (7%) annually

Improved soil, water, and air quality

Reference: http://onlinelibrary.wiley.com/doi/10.1002/bbb.1728/pdf

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

External Advisory Board

USCAR
David Brooks

American Petroleum Institute
Bill Cannella

Fuels Institute
John Eichberger

Truck & Engine Manufacturers Assn
Roger Gault

Advanced Biofuels Association
Michael McAdams

Flint Hills Resources
Chris Pritchard

EPA
Paul Machiele

CA Air Resources Board
James Guthrie

UL
Edgar Wolff-Klammer

University Experts
Ralph Cavalieri (WSU, emeritus)
David Foster (U. Wisconsin, emeritus)

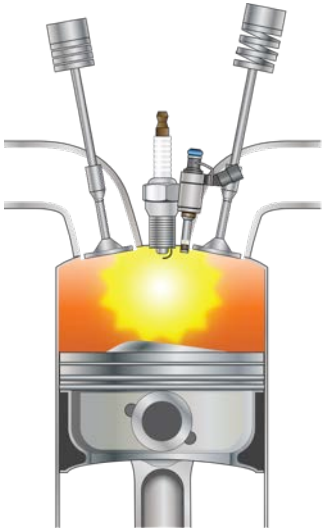
Industry Expert
John Wall (Cummins, retired)

Co-Optima Scope

- Focusing only on liquid fuels
- Identify blendstocks to blend into petroleum base fuel
- Considering only non-food-based biofuel feedstocks
  Assessing WTW emissions for biofuel options (GHG, water, etc)
- Considering hybridized/non-hybridized solutions
- Provide data, tools, and knowledge to stakeholders – objective is not to “pick winners”

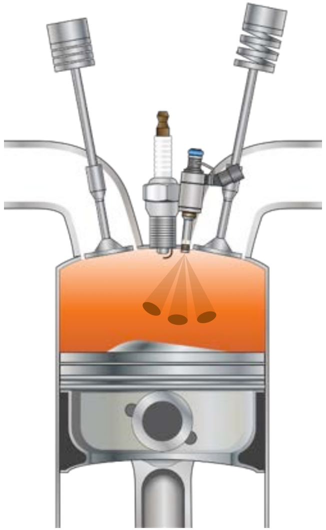
Two Parallel R&D Projects

Light-Duty



Boosted SI

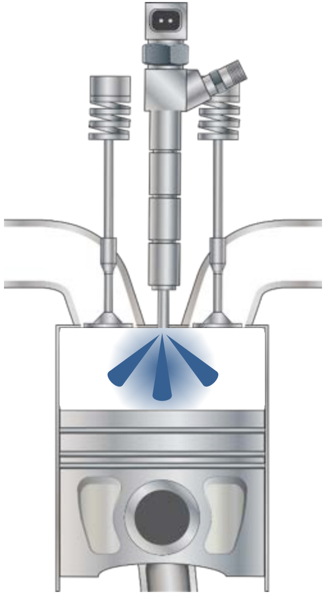
Near-term



Multi-mode SI/ACI

Mid-term

Medium/Heavy-Duty



Mixing Controlled

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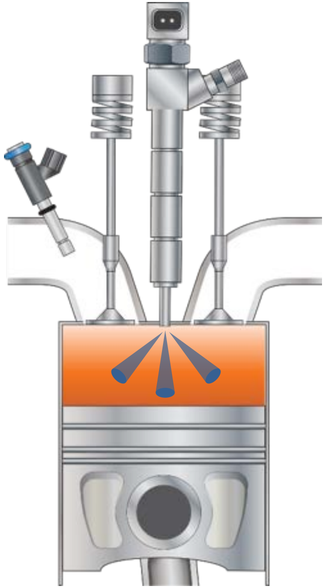
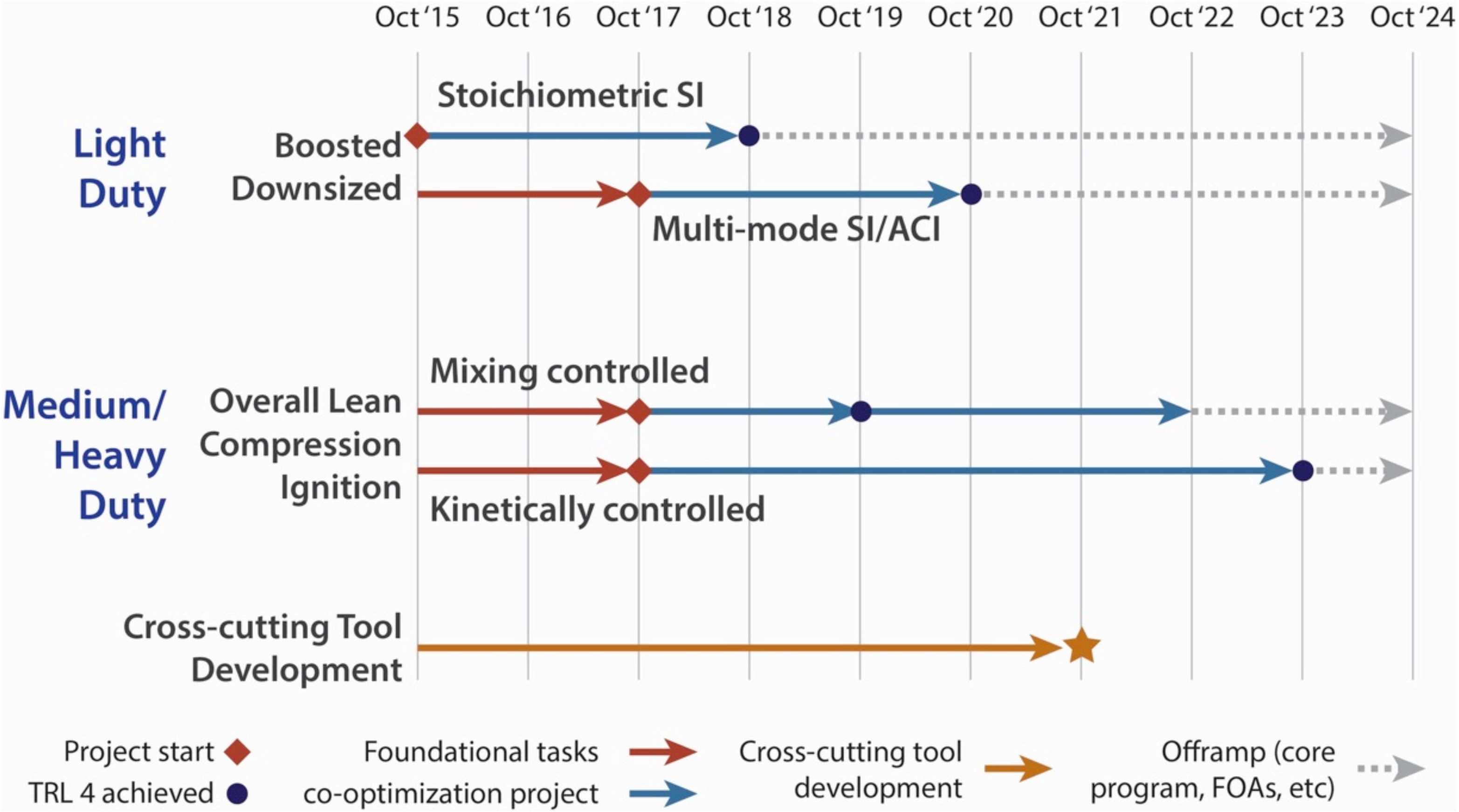


Kinetically Controlled

Longer-term

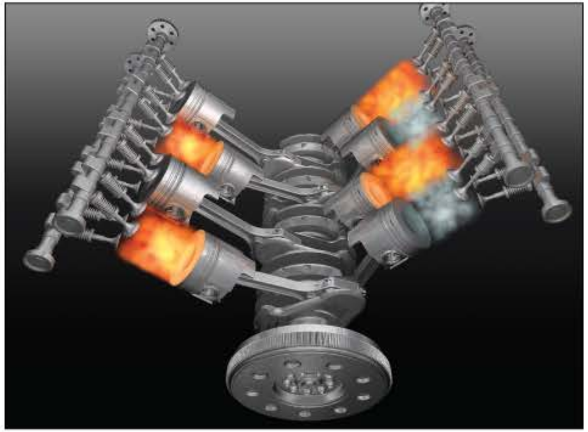
Timeline



Oct '15
Oct '16
Oct '17
Oct '18
Oct '19
Oct '20
Oct '21
Oct '22
Oct '23
Oct '24
Light Duty
Stoichiometric SI
Boosted Downsized
Multi-mode SI/ACI
Medium/ Heavy Duty
Mixing controlled
Overall Lean Compression Ignition
Kinetically controlled
Cross-cutting Tool Development
Project start
TRL 4 achieved
Foundational tasks
co-optimization project
Cross-cutting tool development
Offramp (core program, FOAs, etc)

Foundational Technical Questions

What fuels do engines *really* want?



What fuels *should* we make?

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

Theoretical foundation: “merit function”

Engine efficiency can be expressed as a product of various “efficiencies”:

$$\eta_{th} = \eta_{ideal} * \eta_{glh} * \eta_{comb} * \eta_{pump} * \eta_{ht} * \eta_{emiss} \cdots$$

$$\eta_{ideal} = 1 - \frac{1}{CR^{\gamma-1}}$$

η_{glh} = combustion phasing (“degree of constant V combustion”)

η_{comb} = combustion efficiency

η_{pump} = pumping losses

η_{ht} = heat transer losses

η_{emiss} = emission control losses

Theoretical foundation: "merit function"

Since we are interested in relative efficiency, we can differentiate to get:

$$\frac{d\eta_{th}}{\eta_{th}} = \frac{d\eta_{CR}}{\eta_{CR}} + \frac{d\eta_{\gamma}}{\eta_{\gamma}} + \frac{d\eta_{glh}}{\eta_{glh}} + \frac{d\eta_{comb}}{\eta_{comb}} + \frac{d\eta_{pump}}{\eta_{pump}} + \frac{d\eta_{ht}}{\eta_{ht}} + \frac{d\eta_{emiss}}{\eta_{emiss}} + \ldots$$

PMI, $T_{c,90}$

HOV

Flame Speed

RON, octane sensitivity, HOV

How can we relate these terms to fuel properties?

Efficiency merit function approach

Octane Index

Charge Cooling

RON

Octane Sensitivity

Heat of Vaporization

$$\text{Merit} = \alpha \bullet f(\text{RON}) + \beta \bullet f(K, S) + \gamma \bullet f(\text{HOV})$$

$$+ \varepsilon \bullet f(S_L) + \zeta \bullet f(\text{PMI}) + \eta \bullet f(T_{c,90,conv})$$

Flame Speed

PM Emissions

Catalyst Light-off Temp (cold start)

Dilution Tolerance

Emissions Penalties

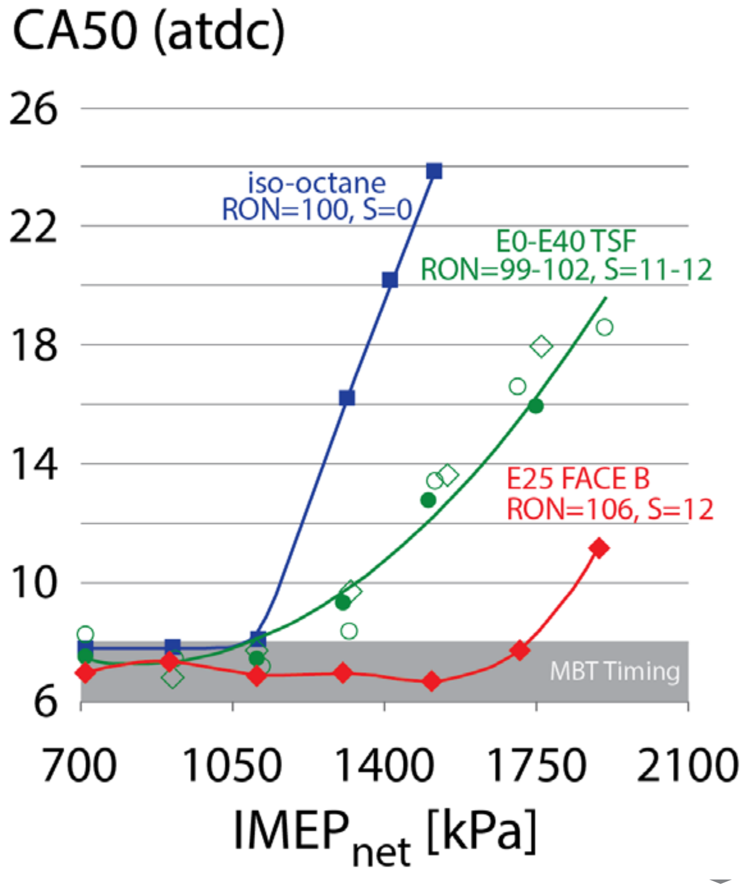
Efficiency merit function approach

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

Technical report with details being published September 2017

Decoupling S and HOV impacts

- With DI, increasing S from 0 to ~ 11 at RON=100 yields more than half the combustion phasing advance of RON 106, S~12 fuel
- All RON 100, S~11 fuels have similar knock-limited performance gains over ic8: no evident HoV benefit

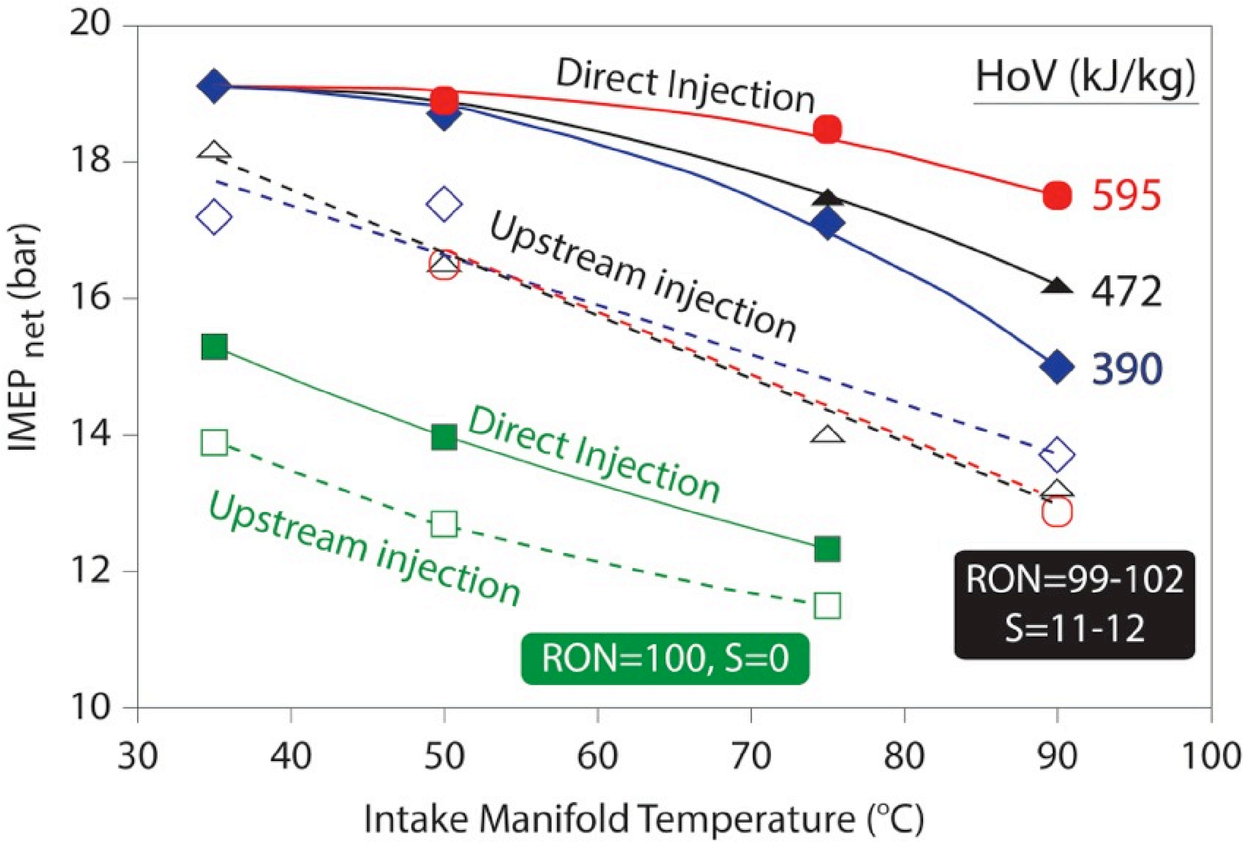


Experimental details: Single cylinder version of GM Ecotec 2.0L, 9.2: CR; side-mounted DI or upstream fuel injection; load sweeps at an intake manifold temp of 50 ^{o} C; sweep intake manifold T for max load at 2 different CA50 phasing

HoV can be important for DI at high intake T

Upstream injected (UI) 100 RON, S ≈ 11 fuels have higher peak IMEP at constant CA50 than iso-octane (RON 100, S =0), and HoV has little effect (S is dominant)

- Direct injection (DI) of iso-octane has HoV benefit, but less than S ≈ 11 effect
- DI of S ≈ 11 fuels also has HoV benefit, which increases with manifold temp.



Question 2: What fuels should we make?

Approach:

Identify blendstock options that provide key properties

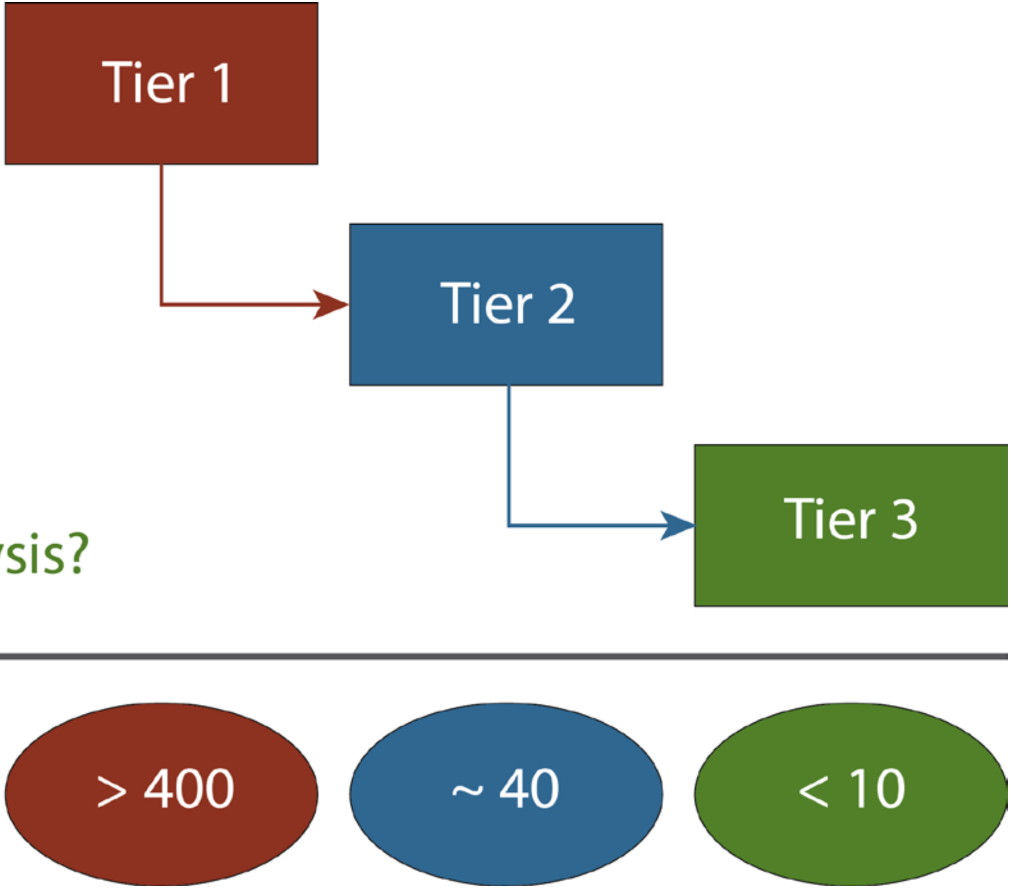
Tiered blendstock identification

Can it be a fuel blendstock?

Does it provide desired performance?

Does it merit focused experiments and analysis?

blendstocks:



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

Present in commercial fuels:

- Hydrocarbons
  - Normal paraffins
  - Iso-paraffins
  - Cycloparaffins
  - Olefins
  - Aromatics
  - Multi-ring aromatics
- Alcohols

Not present in commercial fuels:

- Furans
- Ethers
- Carbonyls
  - Ketones
  - Aldehydes
- Esters
  - Volatile fatty acid esters
  - Fatty esters
- Carboxylic Acids

A major goal of Co-Optima is to conduct a comprehensive and consistent survey of blendstock options:

What blendstocks are able to increase boosted SI performance?

Tiered blendstock identification

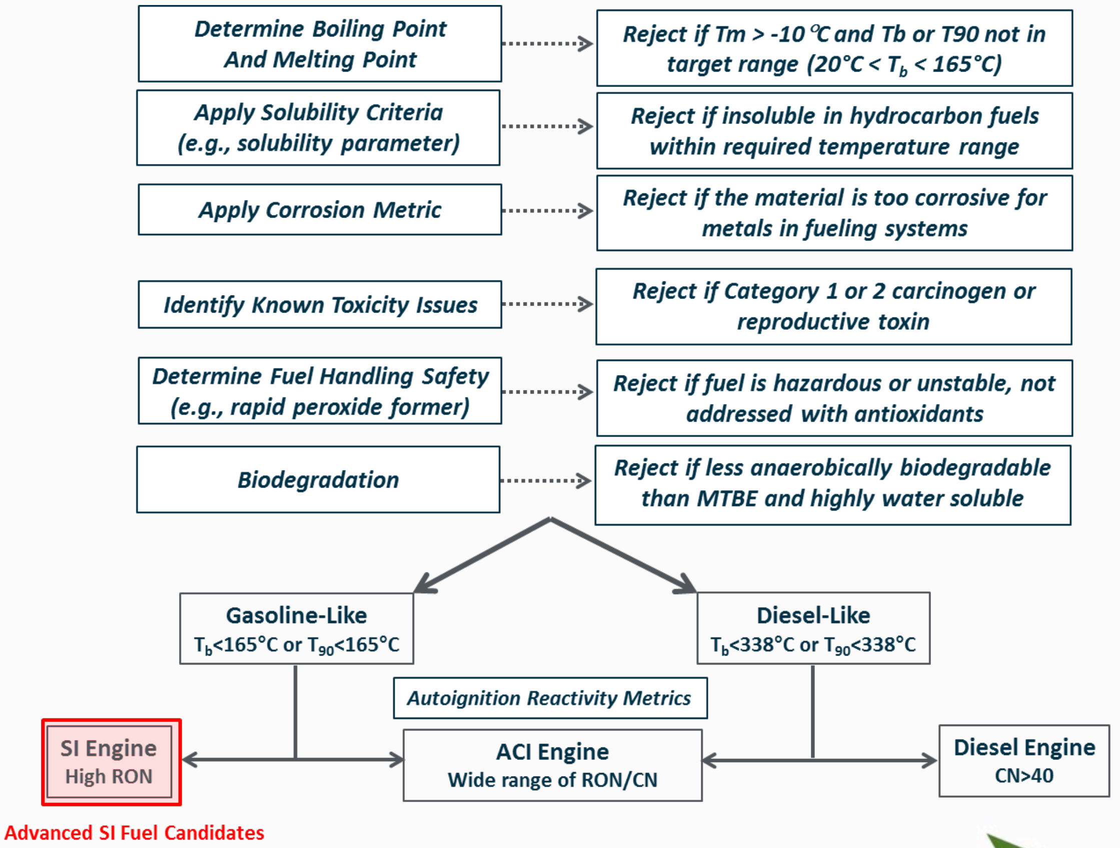
Tier 1

> 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



Tier 1 blendstock screening

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

Tier 2

41 blendstocks

10 chemical families

Measure blendstock properties

Evaluate blendstock performance in BOBs at 10-30% blend levels

Remove candidates from list if improved data indicate they do not meet criteria

Add new candidates as our understanding improves of how fuel structure impacts key properties

Tier 3

Which blendstocks merit comprehensive, consistent, and rigorous study and analysis?

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

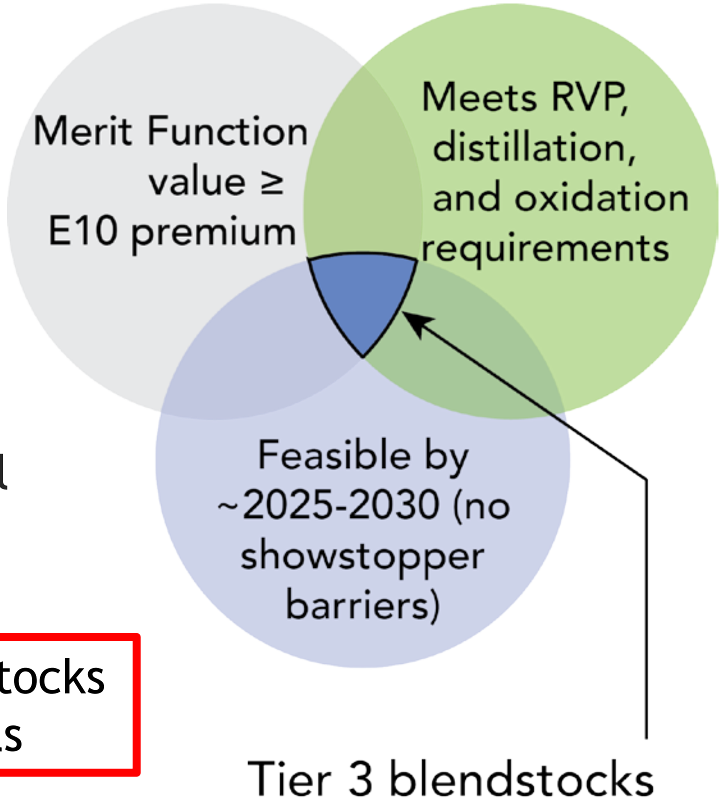
Branched alkanes	
34	2,2,3-Trimethylbutane

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

Tier 2 to Tier 3 transition criteria

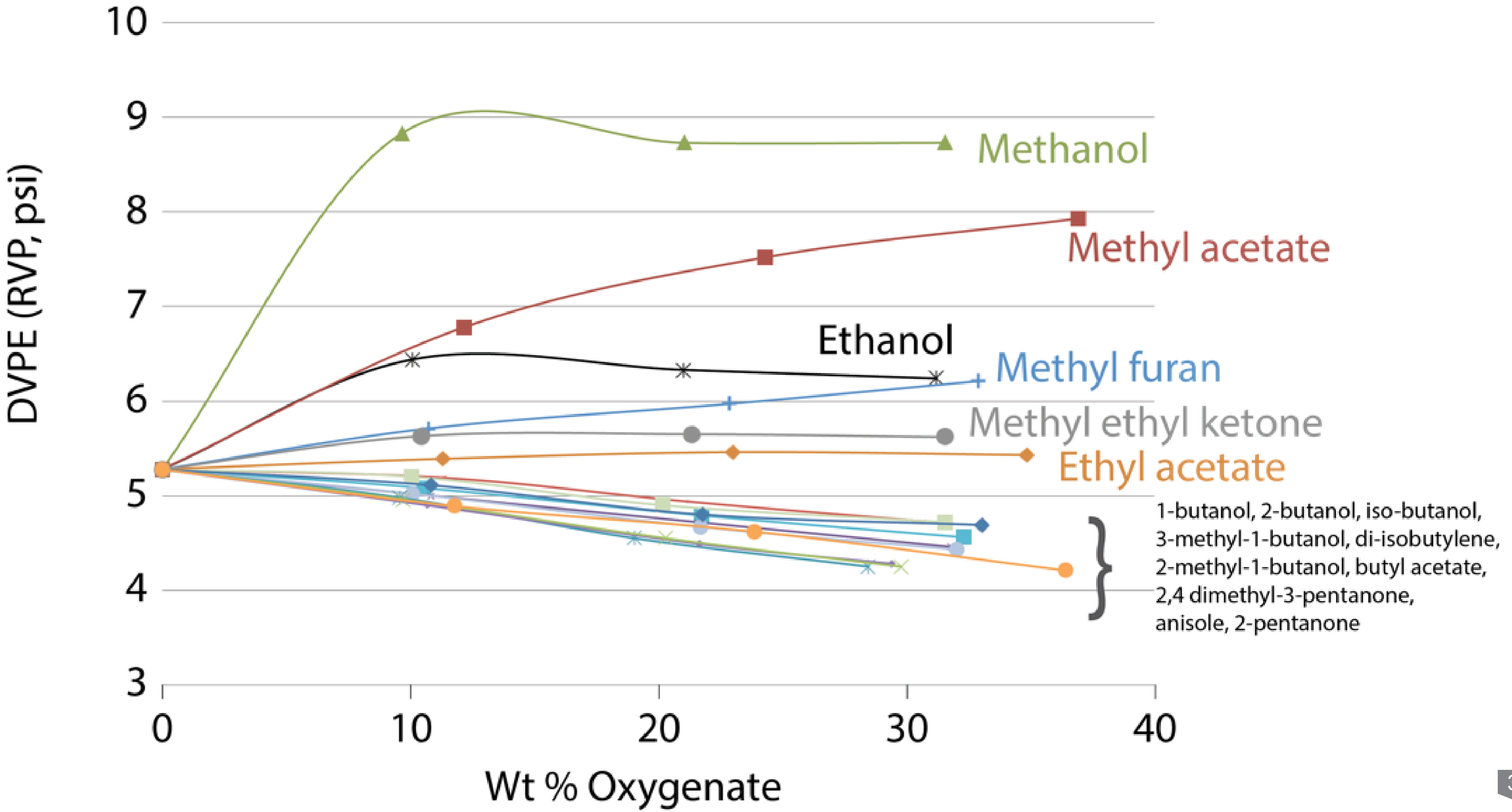
1. Achieve merit function score ≥ E10 premium when blended in petroleum BOB*
2. Meet current critical fuel specs (RVP, distillation, oxidative stability, etc.) when blended in petroleum BOB*
3. No “showstopper” barriers
   - Candidates must have viable path to potential market introduction by ~2025 –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



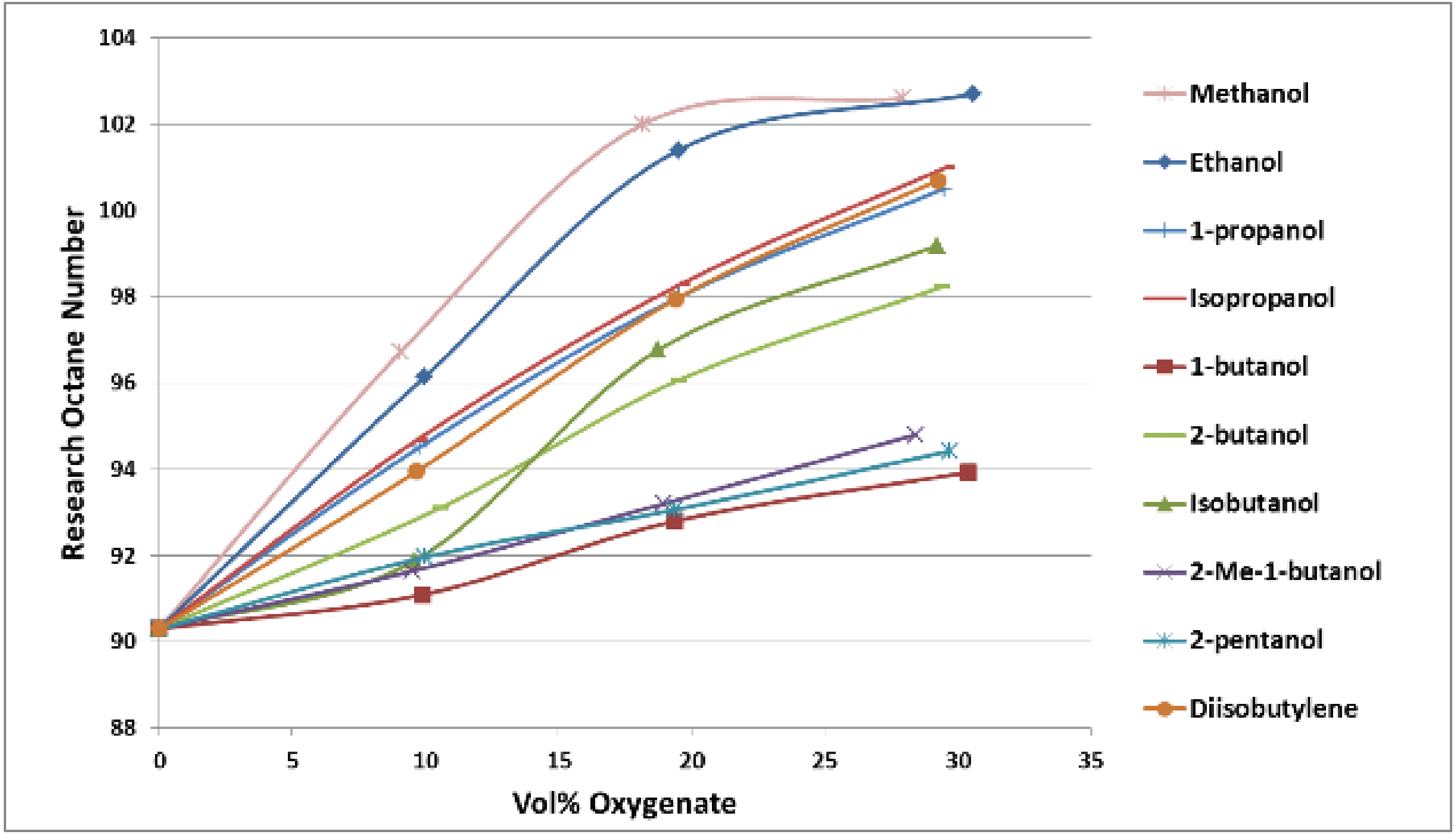
Tier 2->3 transition allows focused effort on blendstocks with greatest potential to meet Co-Optima goals

* BOB = blendstock for oxygenate blending; evaluated at blend levels of 10, 20, and 30% by volume

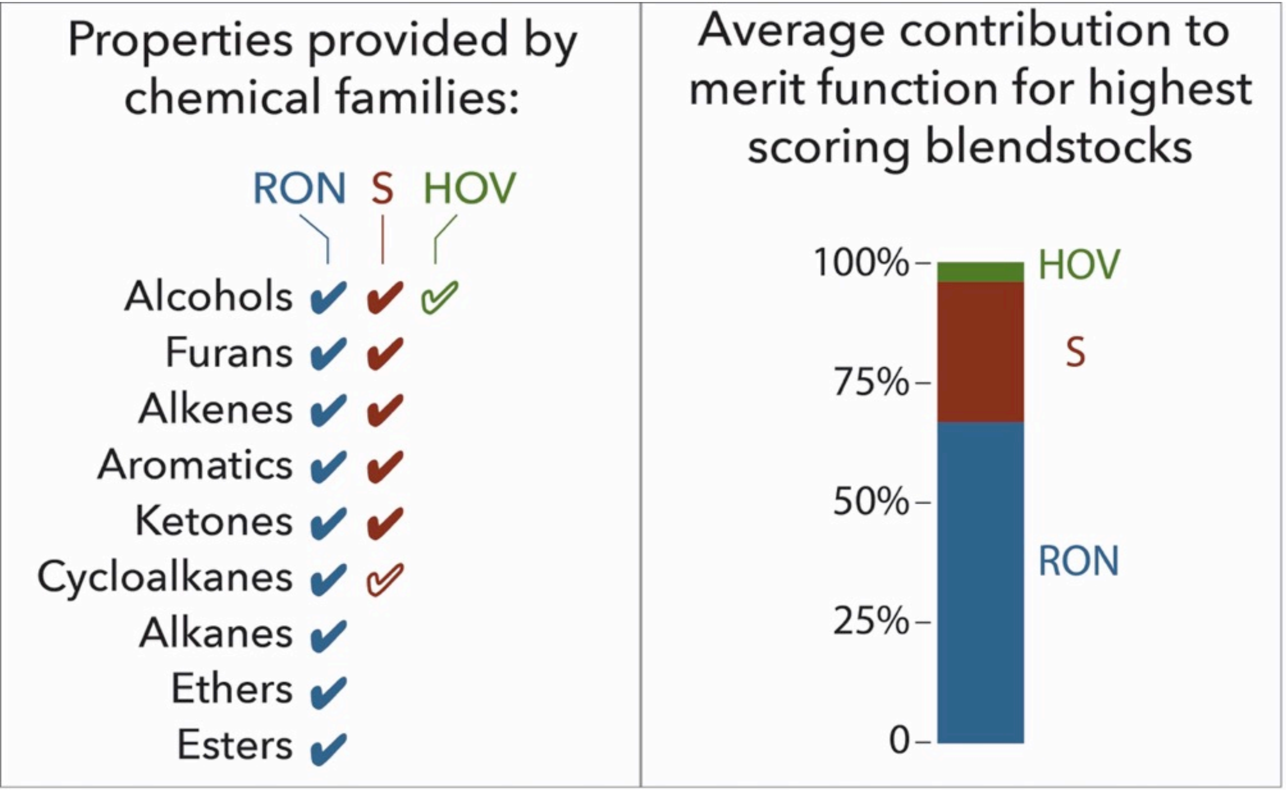
Example blendstock data: RVP



Determining blending behavior



High-potential blendstocks identified



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

Question 3: What will work in the real world?

Approach:

Conduct comparative, systems-level analyses of economic, environmental, state of technology, and market factors

Assess likelihood of commercial scale impact by 2025-2030

Analysis Metrics

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

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

Assessed for both fossil and renewable blendstocks (Market)

Screening assessment results

	Technology readiness							Economics					Environmental					Infrastructure compatibility, etc					
	SOT-fuel	SOT-vehicle	Conversion TRL	Feedstock quality	# viable routes	Feedstock sensitivity	Process robustness	Target cost	Cost reduction	Coproducts	Blendstock competition	Feedstock cost	Carbon efficiency	Yield	Life cycle GHG	Life cycle FE consumption	Life cycle water	Infrastructure compatibility	Regulatory requirements	Vehicle compatibility	Political factors	Geographic factors	Uncertainty
Ethanol	Favorable	Favorable	Favorable	Favorable	Neutral	Neutral	Neutral	Neutral	Favorable	Favorable	Favorable	Favorable	Neutral	Unfavorable	Favorable	Favorable	Neutral	Neutral	Favorable	Unfavorable	Favorable	Favorable	Favorable
Methanol	Favorable	Neutral	Favorable	Favorable	Unfavorable	Neutral	Neutral	Favorable	Favorable	Favorable	Favorable	Favorable	Neutral	Favorable	Favorable	Favorable	Neutral	Neutral	Neutral	Unfavorable	Unfavorable	Unfavorable	Unfavorable
1-Butanol	Neutral	Insufficient data	Neutral	Favorable	Neutral	Neutral	Neutral	Favorable	Favorable	Unfavorable	Neutral	Favorable	Unfavorable	Unfavorable	Neutral	Favorable	Neutral	Favorable	Favorable	Neutral	Neutral	Neutral	Unfavorable
2-methyl butanol	Unfavorable	Insufficient data	Unfavorable	Favorable	Neutral	Neutral	Neutral	Unfavorable	Unfavorable	Favorable	Favorable	Favorable	Unfavorable	Neutral	Unfavorable	Favorable	Neutral	Favorable	Neutral	Neutral	Unfavorable	Neutral	Unfavorable
2-Butanol	Unfavorable	Insufficient data	Unfavorable	Favorable	Neutral	Neutral	Neutral	Neutral	Unfavorable	Favorable	Favorable	Favorable	Unfavorable	Neutral	Neutral	Favorable	Neutral	Favorable	Neutral	Neutral	Neutral	Favorable	Neutral
iso-Butanol	Favorable	Insufficient data	Neutral	Neutral	Neutral	Neutral	Neutral	Neutral	Favorable	Favorable	Favorable	Favorable	Unfavorable	Neutral	Neutral	Favorable	Neutral	Favorable	Favorable	Neutral	Favorable	Favorable	Neutral
Guerbet alcohols	Favorable	Insufficient data	Neutral	Favorable	Neutral	Neutral	Neutral	Neutral	Favorable	Favorable	Neutral	Favorable	Neutral	Neutral	Favorable	Favorable	Neutral	Neutral	Insufficient data	Neutral	Neutral	Insufficient data	Neutral
Furan mixture	Unfavorable	Insufficient data	Unfavorable	Favorable	Neutral	Neutral	Neutral	Neutral	Neutral	Favorable	Favorable	Favorable	Neutral	Favorable	Neutral	Favorable	Neutral	Unfavorable	Neutral	Neutral	Unfavorable	Favorable	Unfavorable
Methyl acetate	Favorable	Insufficient data	Unfavorable	Favorable	Neutral	Neutral	Neutral	Favorable	Favorable	Favorable	Neutral	Favorable	Favorable	Favorable	Favorable	Favorable	Neutral	Neutral	Neutral	Neutral	Unfavorable	Neutral	Unfavorable
Ethyl acetate	Neutral	Insufficient data	Unfavorable	Favorable	Neutral	Neutral	Neutral	Unfavorable	Favorable	Favorable	Neutral	Favorable	Unfavorable	Unfavorable	Favorable	Favorable	Neutral	Neutral	Neutral	Neutral	Neutral	Favorable	Unfavorable

Legend: Favorable · Neutral · Unfavorable · Insufficient data

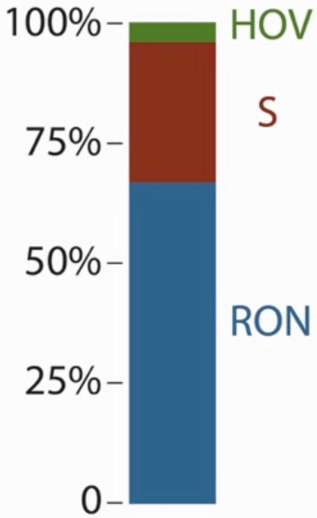
Gasification/catalysis | Fermentation | Hydrolysis/catalysis | Pyrolysis

High-potential blendstocks identified

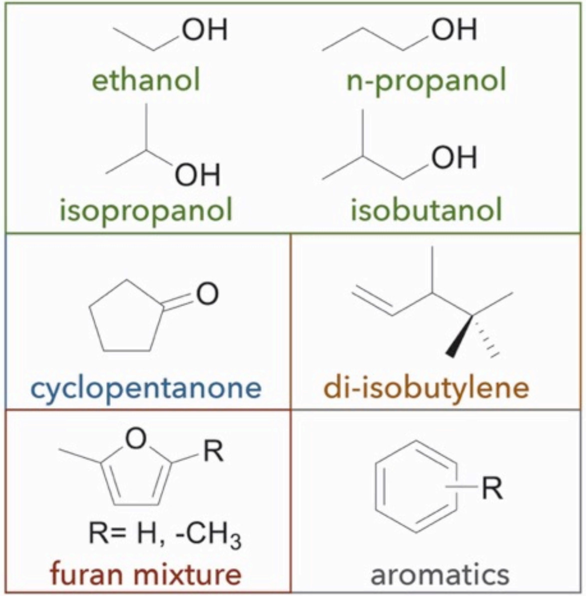
Properties provided by chemical families:

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

Average contribution to merit function for highest scoring blendstocks



Eight representative blendstocks selected for more detailed evaluation



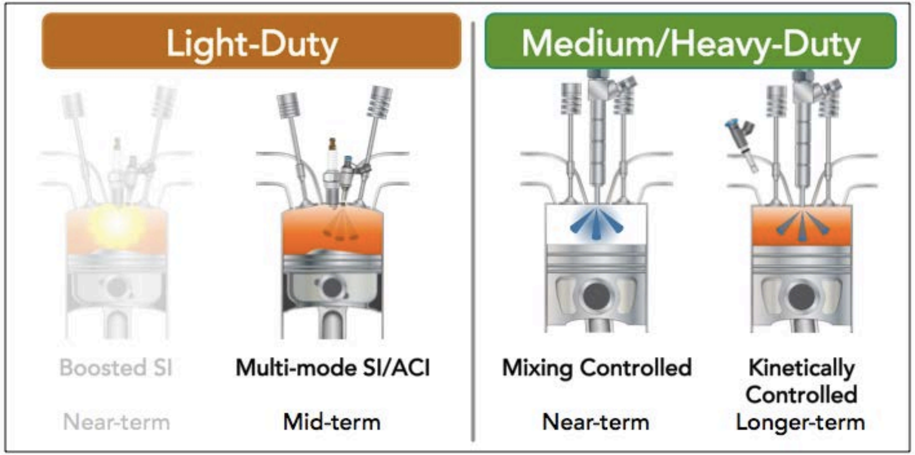
RON = Research octane number ; S = Sensitivity (S = RON – MON) ; HOV = heat of vaporization

Current boosted SI blendstock efforts

- Refine property measurements, improve blend models, and conduct more detailed compatibility studies
- Conduct engine tests to confirm performance and assess potential to meet FE targets
- Carry out emissions control experiments to assess impacts on efficiency and durability
- Conduct detailed life cycle, techno-economic analyses, and refinery integration studies

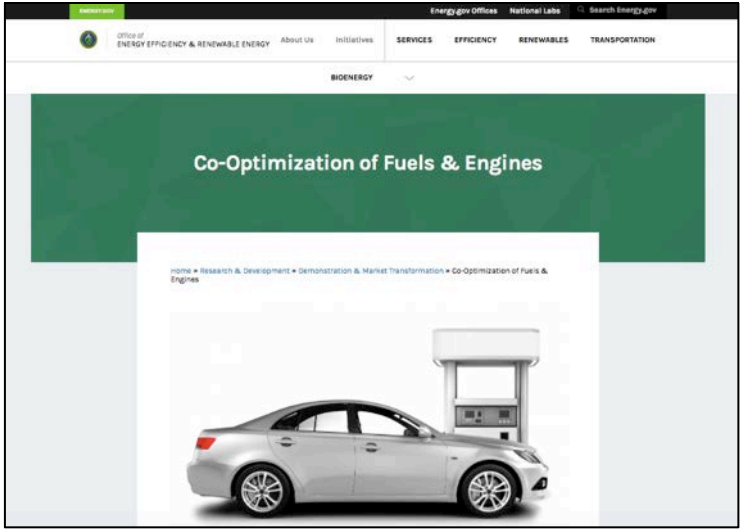
Next steps

- Refine merit function and establish technical basis for advanced gasoline fuel specification for boosted SI by end of FY18
- Conduct more rigorous assessments of Tier 3 candidates
- Assess candidates for potential follow-on scale-up studies
- Expand LD efforts – multi-mode SI-ACI
- Expand MD/HD efforts
- Continue strong engagement with stakeholders to help focus R&D on options that provide "wins" for broad range of stakeholders



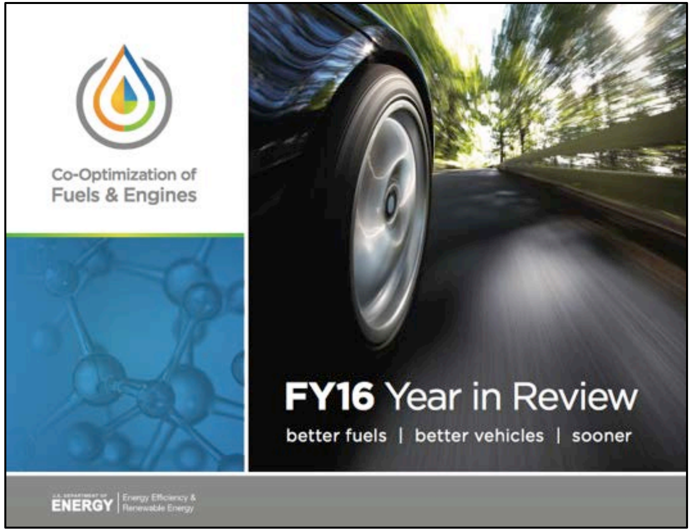
More details

Co-Optima Website



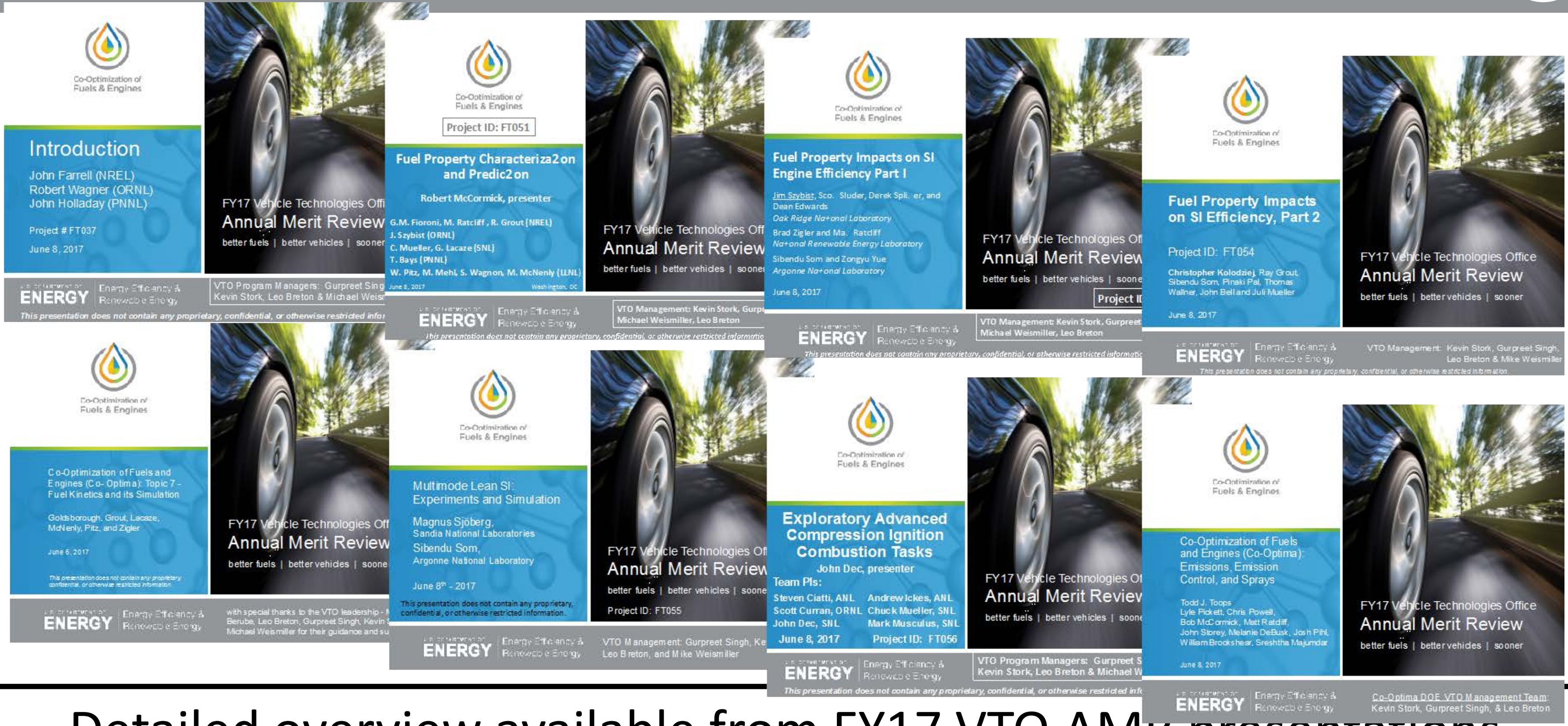
https://energy.gov/eere/bioenergy/co-optimization-fuels-engines

FY 2016 Year in Review Highlights



https://www.nrel.gov/docs/fy17osti/67595.pdf

2017 VTO Peer Review Presentations



Detailed overview available from FY17 VTO AMR presentations

https://www.annualmeritreview.energy.gov

2017 Bioenergy Peer Review Presentations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BIOENERGY

2017 Project Peer Review—Co-Optimization of Fuels and Engines

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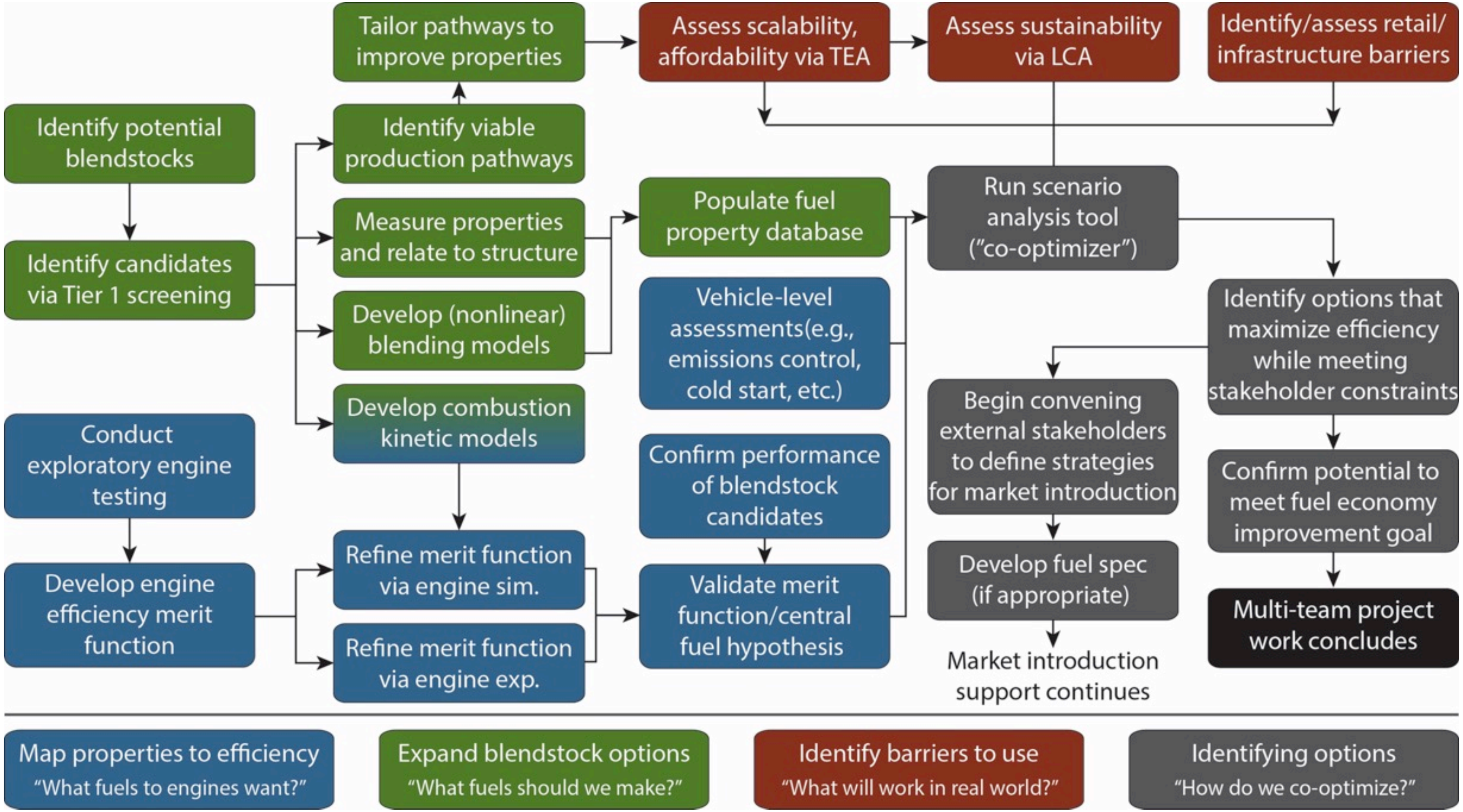
The Bioenergy Technologies Office hosted its 2017 Project Peer Review on March 6-9, 2017, in Denver, Colorado. The presentations from the Co-Optimization of Fuels and Engines sessions are available to view and download below. For detailed session descriptions and presentation titles, view the 2017 Project Peer Review Program Booklet.

- Co-Optima Overview
- High-Performance Fuels
- Analysis of Sustainability, Supply, Economics, Risk and Trade (ASSERT)
- Market Transformation

https://energy.gov/eere/bioenergy/downloads/2017-project-peer-review-co-optimization-fuels-and-engines

Thank You!

Technical Approach



University Partners

Cornell / UCSD
Identify differences in combustion characteristics of diesel/biofuel blends vs petroleum-based fuels

LSU / TAMU / U Conn.
Develop method to characterize alternative fuel candidates and associated models and metrics for predicted engine performance

Univ. Michigan
Develop engine combustion model to simulate key parameters while reducing computational expense 80%

MIT / Univ. Central Florida
Develop detailed kinetic models for several biofuels using an advanced computational approach

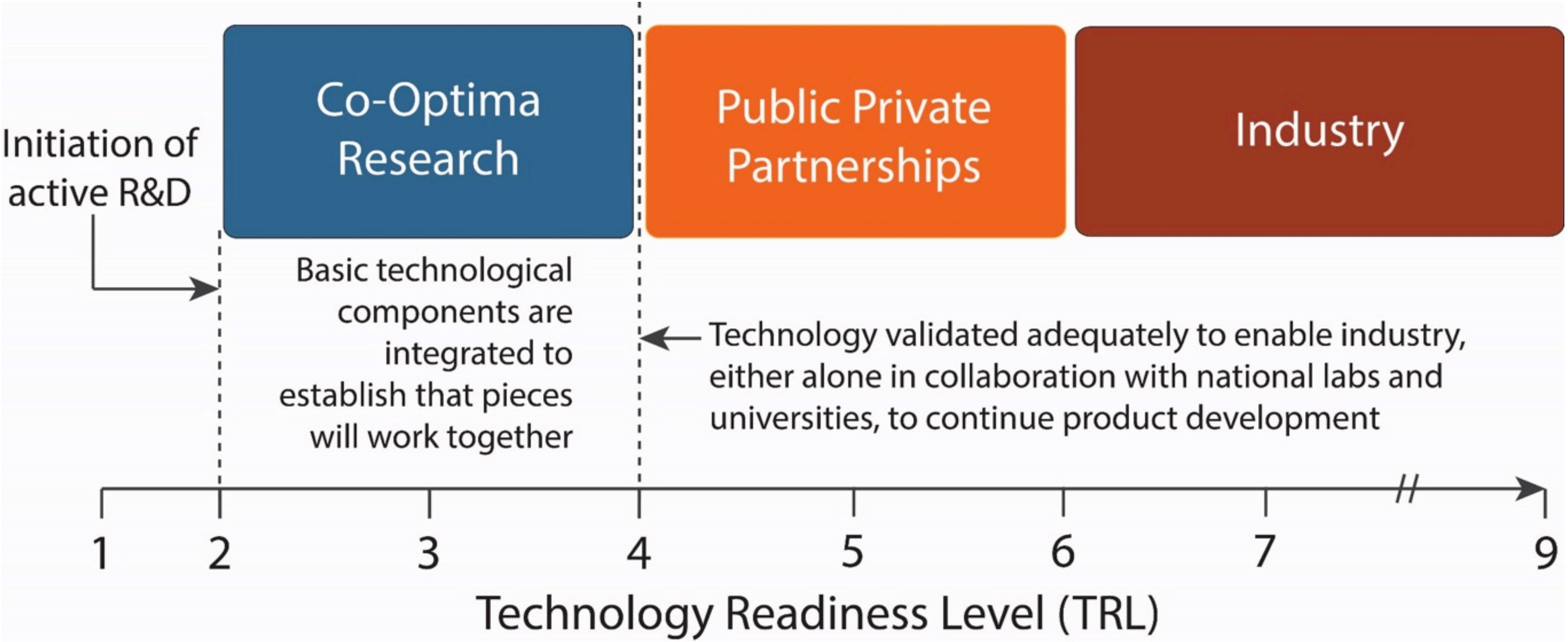
U. Mich. - Dearborn/Oakland U.
Use a miniature ignition screening RCM to study ignition properties/combustion characteristics of alternative fuels.

Yale
Measure sooting tendencies of various biofuels and develop emission indices relevant to real engines

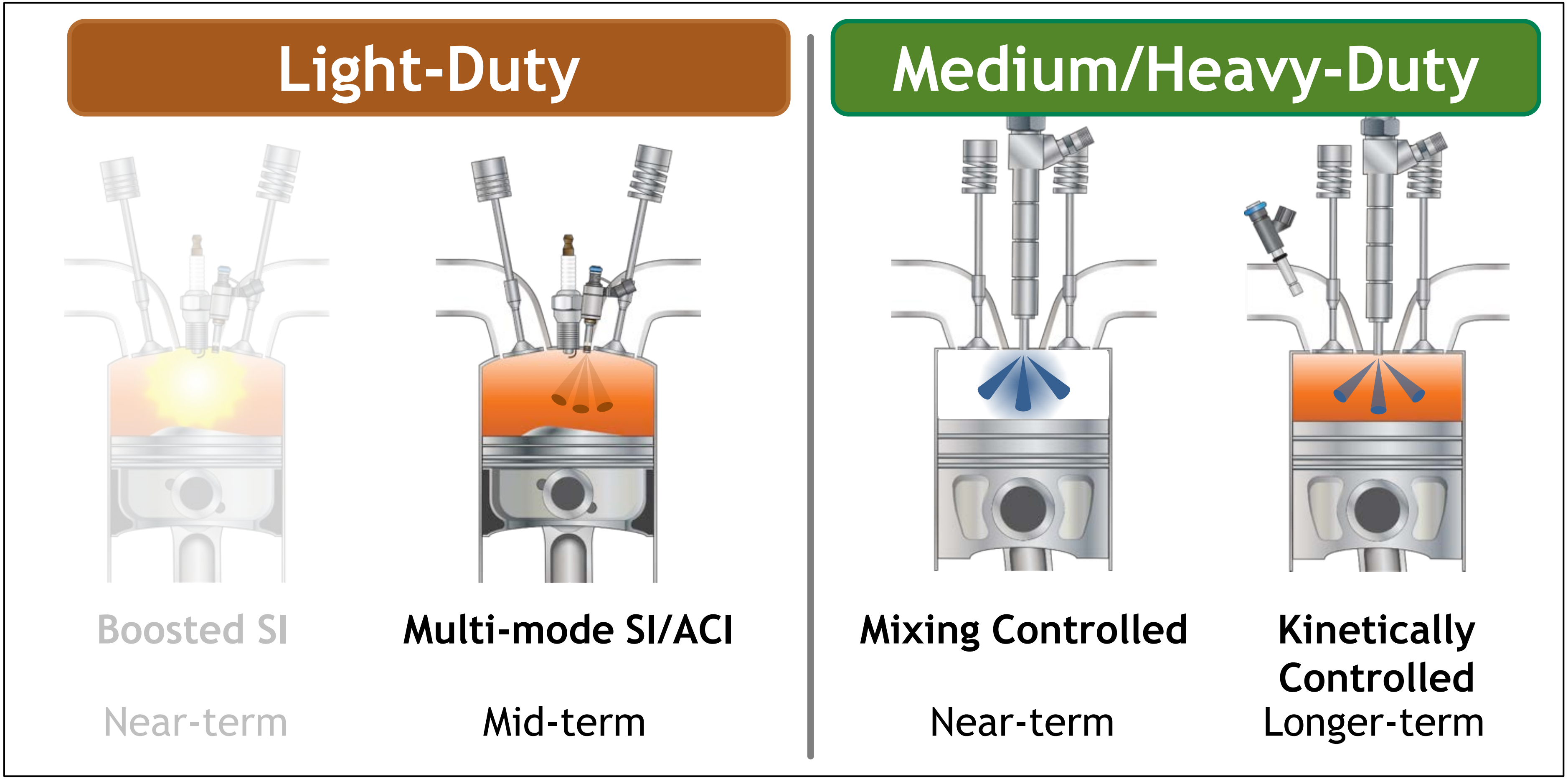
Univ. Alabama
Examine combustion properties of biofuels and blends using advanced diagnostics under realistic ACI engine conditions.

Univ. Central FL/Penn State
Generate fuel characterization data related to fuel spray atomization, flame topology, etc, and compatibility for prioritized fuels

Integration With Industry



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



Light-Duty
Medium/Heavy-Duty
Boosted SI
Near-term
Multi-mode SI/ACI
Mid-term
Mixing Controlled
Near-term
Kinetically Controlled
Longer-term

Fuel property database*

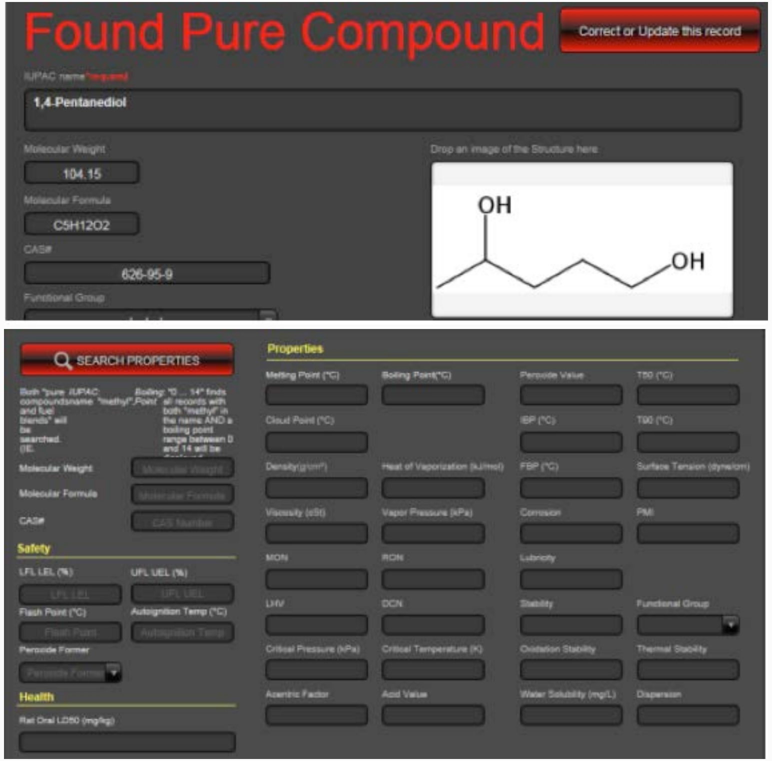
Tier 1

> 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



* Publicly accessible: https://fuelsdb.nrel.gov/fmi/webd#FuelEngineCoOptimization

Tier 1 blendstock screening

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