Co-Optimization of Fuels & Engines

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

Recent Progress on Light-duty Boosted Spark-ignition Fuels/Engines

John Farrell (NREL)

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better fuels | better vehicles | sooner

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

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Other Co-Optima Leadership Team Members:

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Goals and Outcomes

Light-duty

Up to 15% fuel economy (FE) improvement*
Phase 1: boosted SI; Phase 2: multi-mode SI/ACI

Heavy-duty

Up to 1-4% FE improvement (worth $1-5B/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

Governing Hypotheses

Central Engine Hypothesis

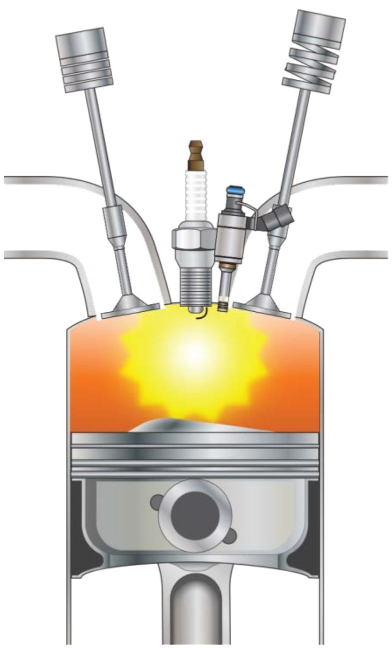
There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range

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

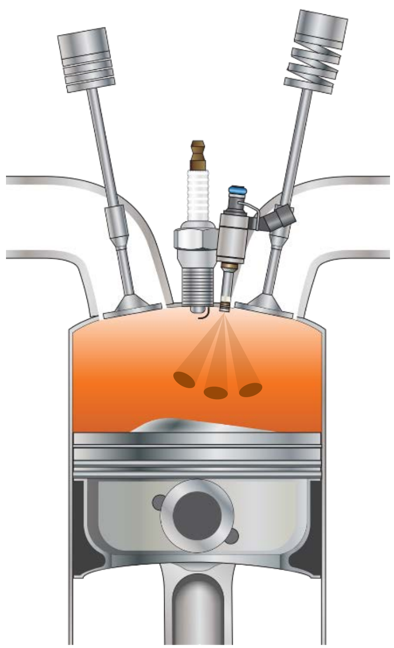
Two Parallel R&D Projects

Light-Duty



Boosted SI

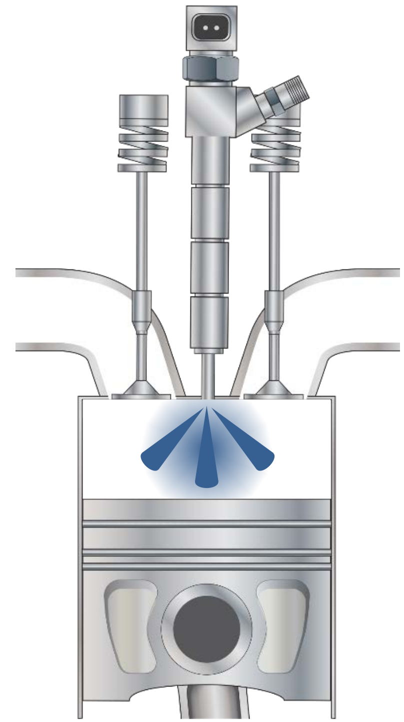
Near-term



Multi-mode SI / ACI

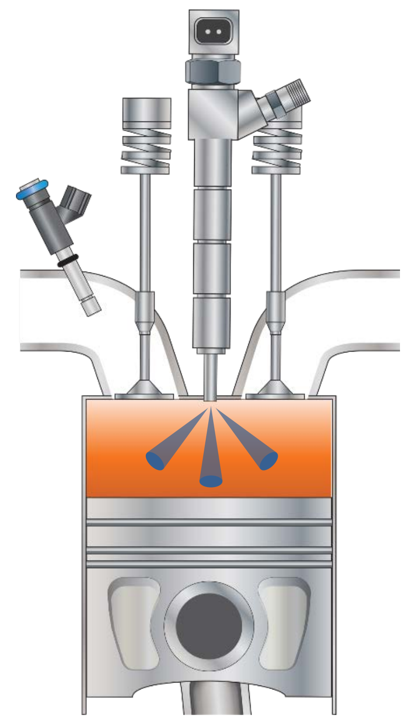
Mid-term

Medium and Heavy-Duty



Mixing Controlled

Near-term



Kinetically Controlled

Longer-term

Co-Optima Team

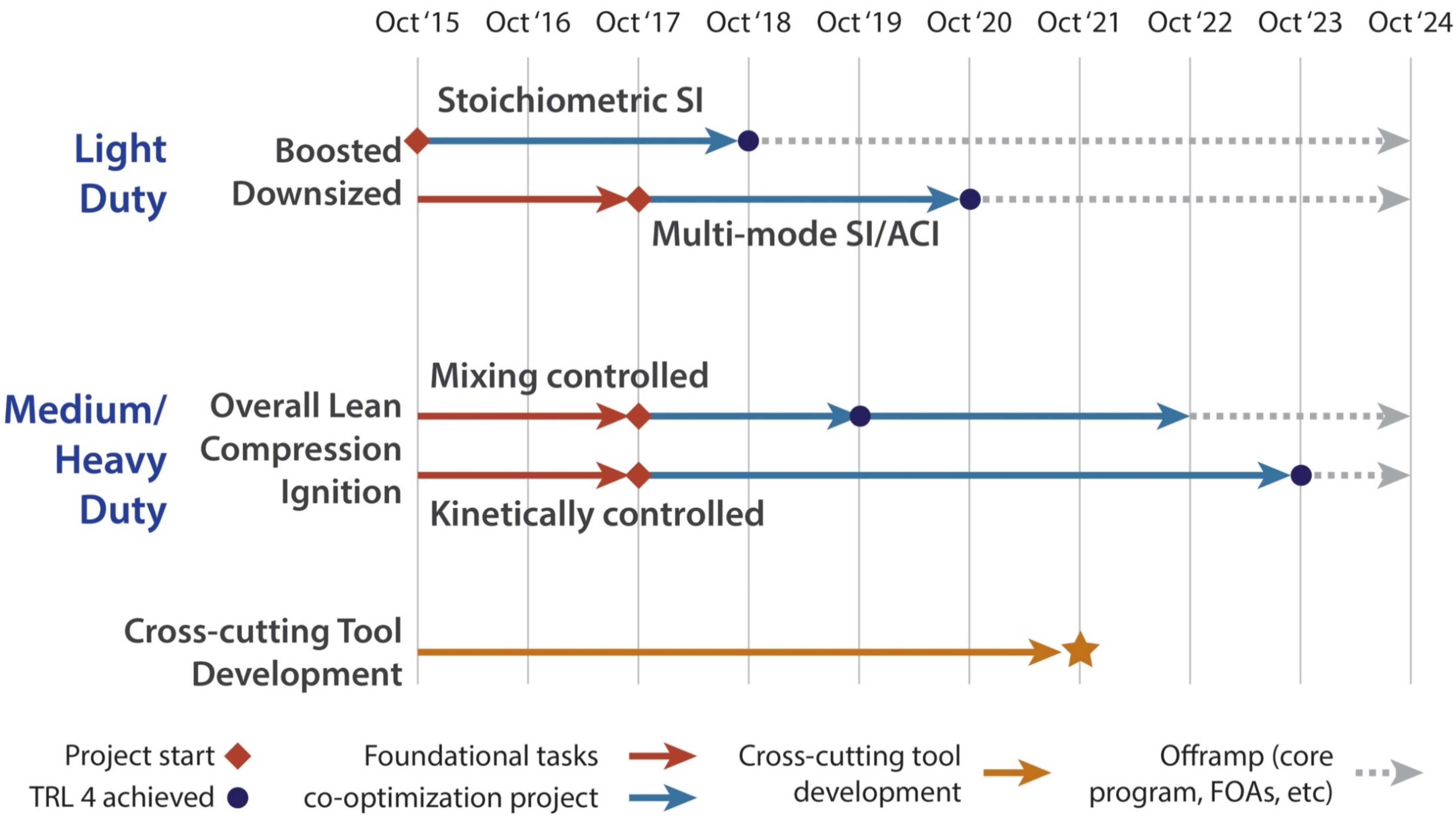
Leveraging expertise and facilities from 9 national labs and 13 universities

External Advisory Board

77 stakeholder organizations

Budget:
FY16: $26M
FY17: $24.5M
Universities: $7M

Timeline



Oct '15
Oct '16
Oct '17
Oct '18
Oct '19
Oct '20
Oct '21
Oct '22
Oct '23
Oct '24
Light Duty
Boosted Downsized
Stoichiometric SI
Multi-mode SI/ACI
Medium/ Heavy Duty
Overall Lean Compression Ignition
Mixing controlled
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)

Overview of approach

Co-Optima is focused on identifying 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

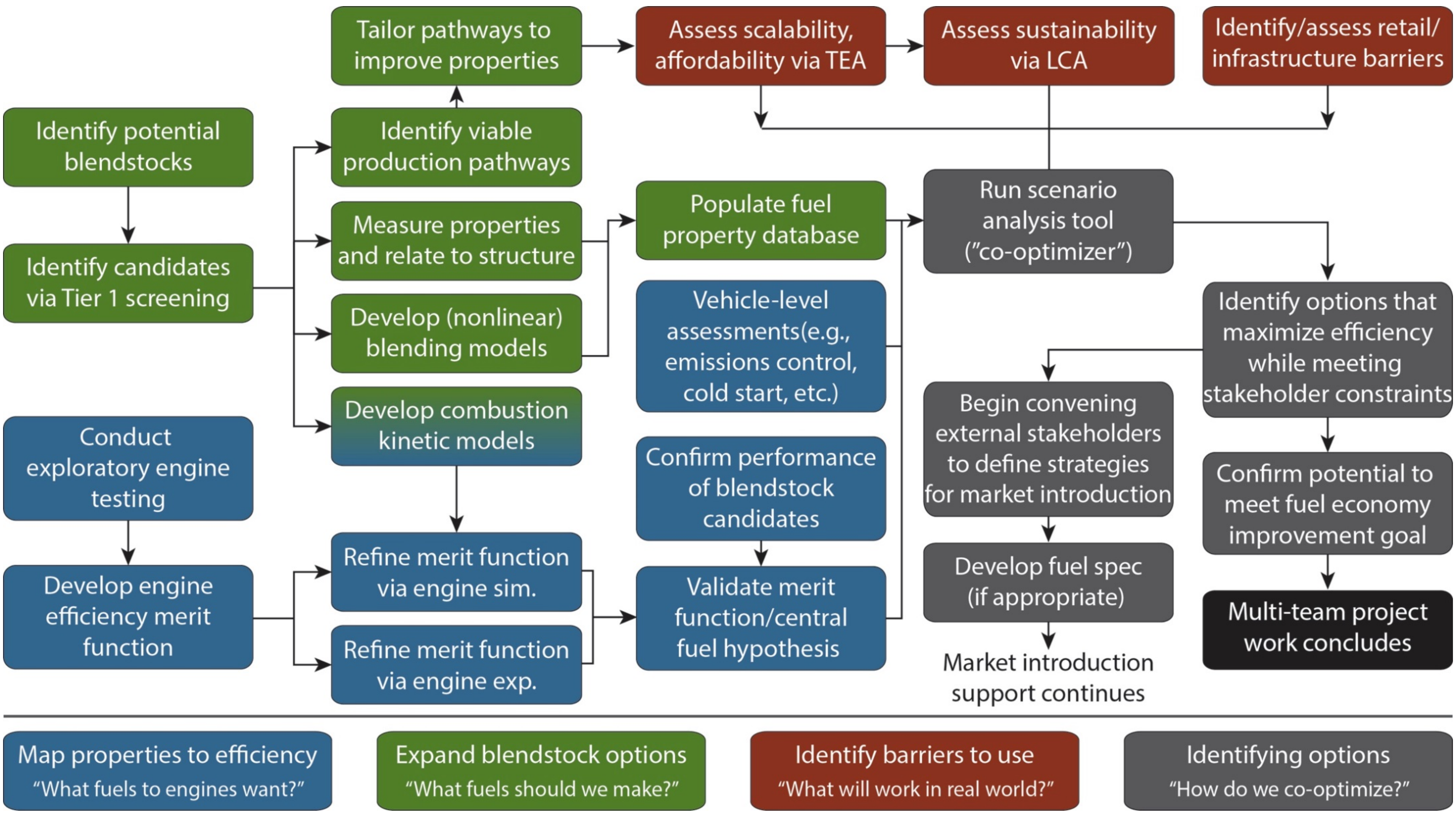
New fuel specs would be analogous to today's gasoline spec, in contrast to (e.g.) E85

However, in support of this, we are pursuing a systematic study of blendstocks to identify a broad range of feasible options

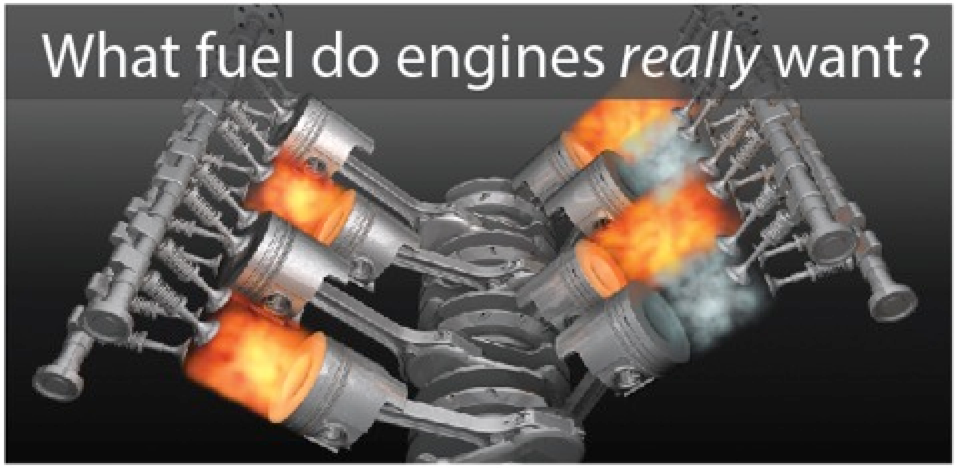
Objective is to identify blendstocks that can provide target ranges of key fuel properties, identify trade-offs on consistent and comprehensive basis, and share information with stakeholders

We are also looking to demonstrate options that can be sourced from biomass while providing technical and societal benefits

Technical Approach



Primary Technical Challenges



Identifying key fuel properties that impact efficiency for advanced spark ignition and compression ignition combustion approaches

Identifying fuel formulations that provide target ranges of key fuel properties when blended with petroleum blendstocks

Technical Challenge 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

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

- RON: $\alpha \bullet f(\text{RON})$
- Octane Sensitivity: $- \beta \bullet f(K, S)$
- Heat of Vaporization: $+ \gamma \bullet f(\text{HOV}) + \delta \bullet f'(\text{HOV})$
- Flame Speed: $+ \varepsilon \bullet f(S_L)$
- PM Emissions: $- \zeta \bullet f(\text{PMI})$
- Catalyst light off T: $- \eta \bullet f(T_{c,90,conv})$

- Merit function establishes fuel property relationships in a systematic and comprehensive way that guides fuel R&D
- Each combustion approach will have unique merit function

Merit Function

$$Merit = \frac{(RON_{mix} - 91)}{1.6} - K\frac{(S_{mix} - 8)}{1.6}$$

$$+ \frac{0.085[ON/kJ/kg_{mix}] \cdot ((HoV_{fuel}/(AFR_{mix}+1)) - (415[kJ/kg]/(14.0[-]+1)))}{1.6}$$

$$+ \frac{((HoV_{mix}/(AFR_{mix}+1)) - (415[kJ/kg]/(14.0[-]+1)))}{15.2} + \frac{(S_{Lmix} - 46[cm/s])}{5.4}$$

$$- H\left(PMI_{mix} - 1.6\right)\left[0.7 + 0.5(PMI_{mix} - 1.4)\right] + 0.008^{\circ}C^{-1}\left(T_{c,90,conv} - T_{c,90,mix}\right)$$

- 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

Fuel Effects on EGR and Lean Dilution Limits

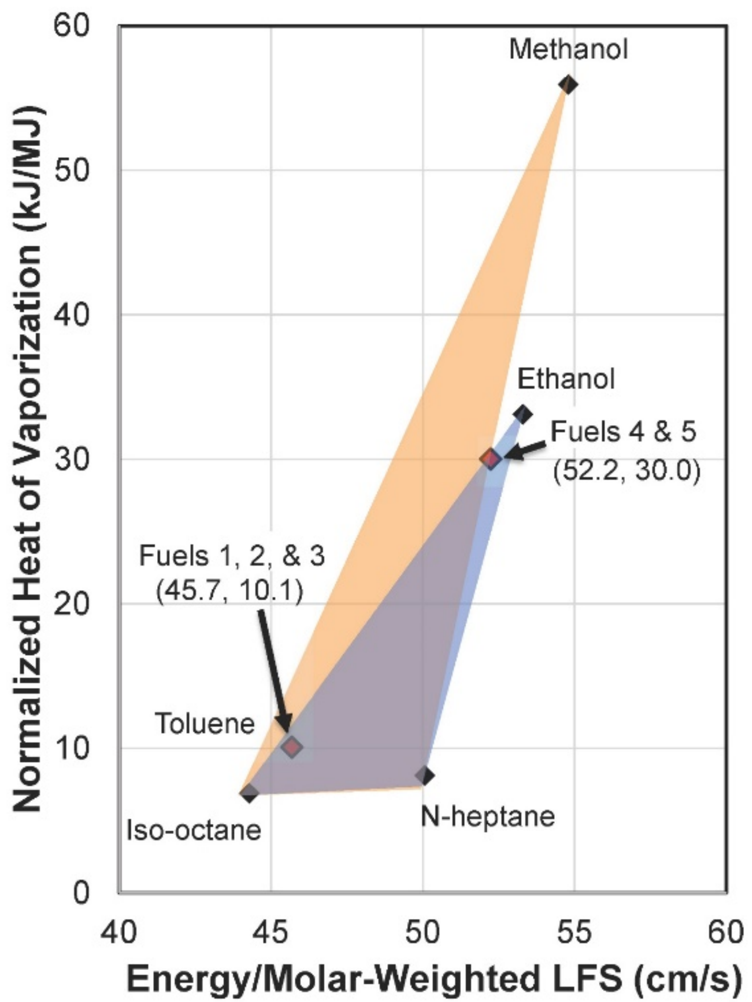
Objective:

- Quantify fuel property effects on increased lean and EGR dilution tolerance compared to engine design parameters

Approach:

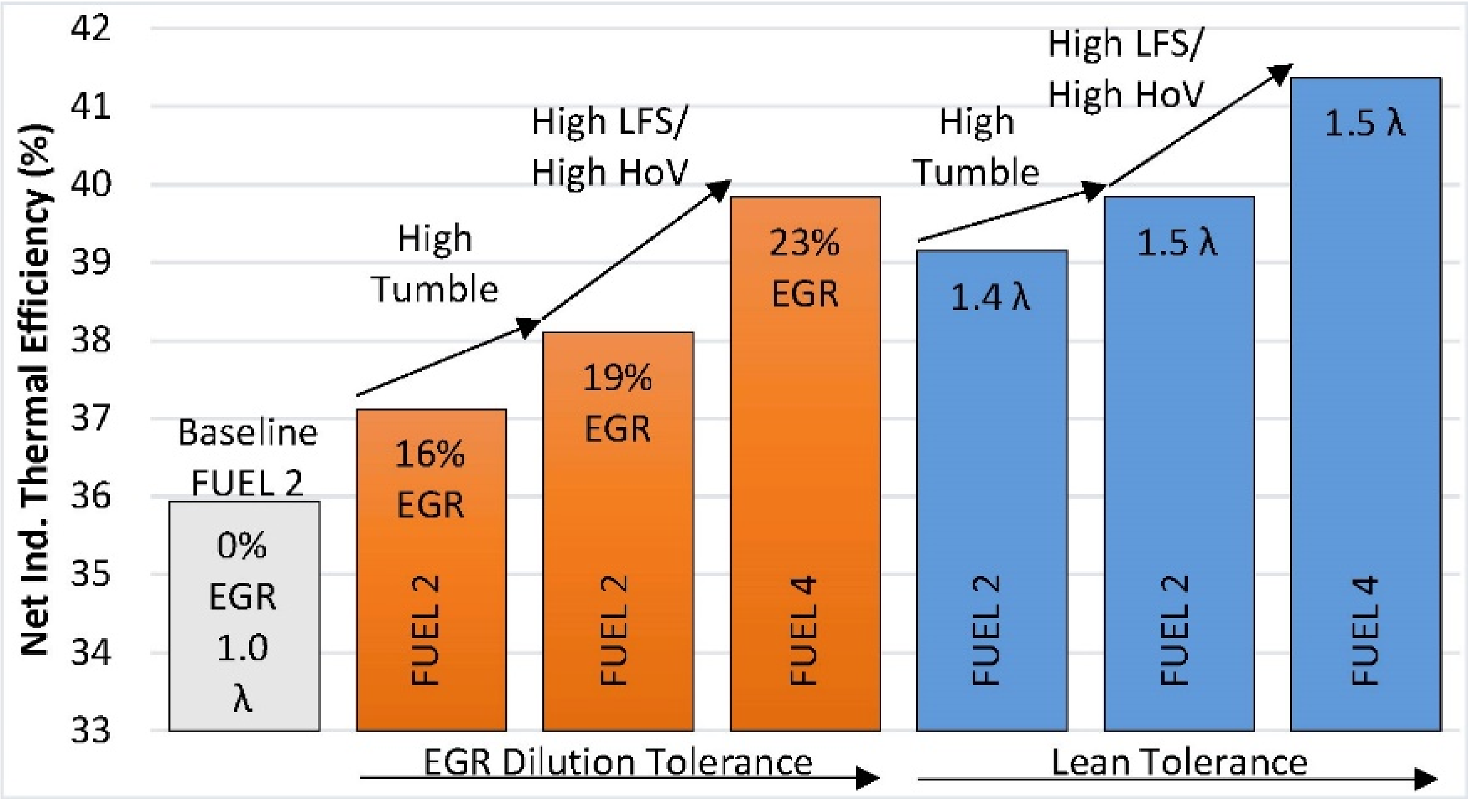
- Test lean and EGR dilution limits of SI combustion with low and high laminar flame speed (LFS) pure component fuel blends

Component	1	2	3	4	5
iso-octane (%wt)		73.6	72.6	7.1	
n-heptane (%wt)		8.7	15.3		35.3
toluene (%wt)	100				
ethanol (%wt)		17.6		92.9	
methanol (%wt)			12.1		64.7



Kolodziej, ANL

Fuel Effects on EGR and Lean Dilution Limits



- Higher LFS Fuels 4/5 showed 2-5% higher EGR tolerance than Fuels 2/3
- Higher tumble ratio (0.6→1.5) showed 2-3% higher EGR tolerance
- **Fuel LFS could extend dilution tolerance as much as engine tumble, increasing engine ITE**
- Under lean conditions, LFS did not consistently increase lean limit, but did increase ITE by 10% shorter combustion duration (2 CAD)

Kolodziej, ANL

Detailed overview: VTO AMR

Detailed overview available from FY17 VTO AMR presentations

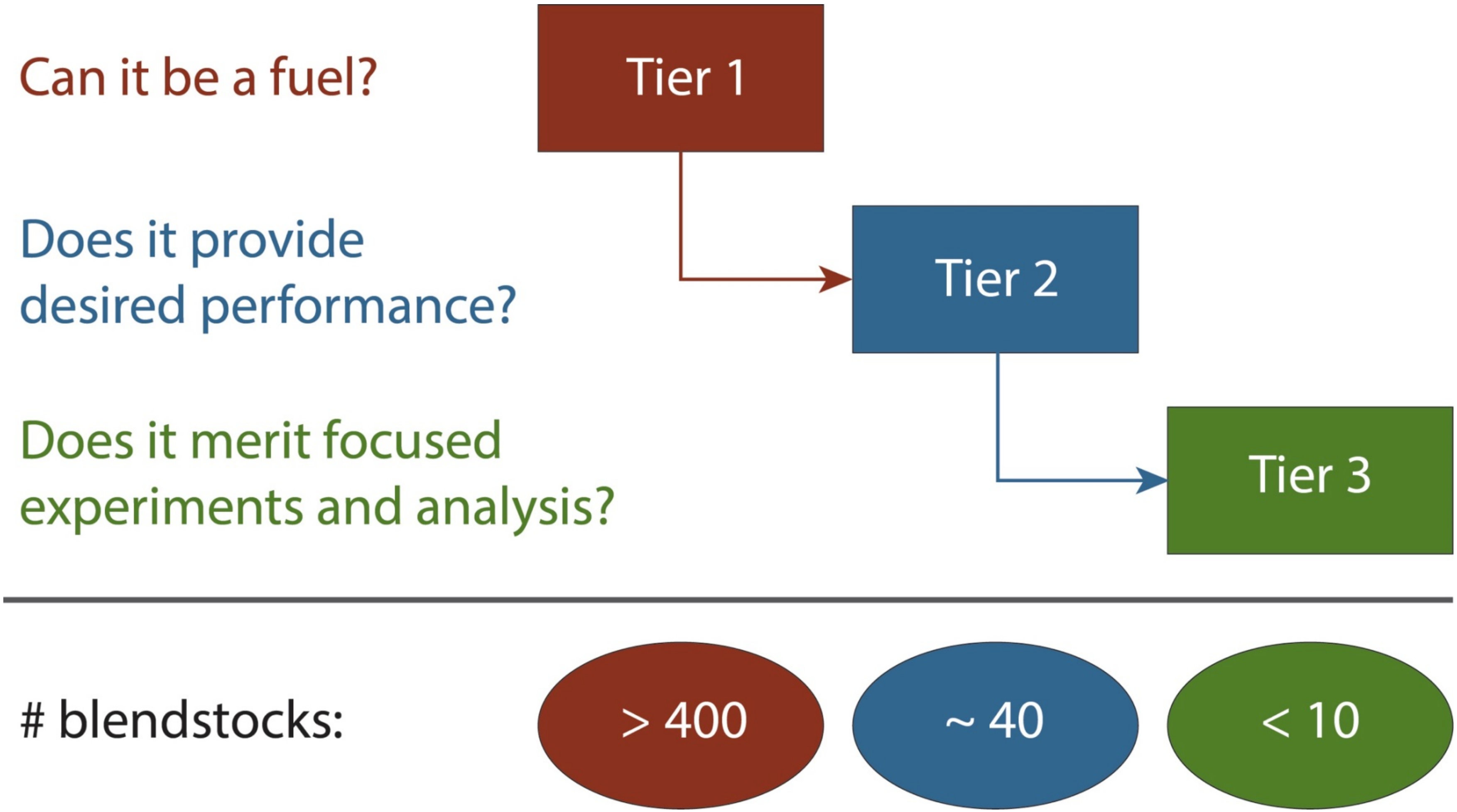
https://www.annualmeritreview.energy.gov

Technical Challenge 2

What fuels should we make?

Identifying blendstock options that provide key properties

Tiered Blendstock Identification



Tiered approach allows efficient prioritization of R&D

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

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

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

Present in commercial fuels

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

Not present in commercial fuels

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

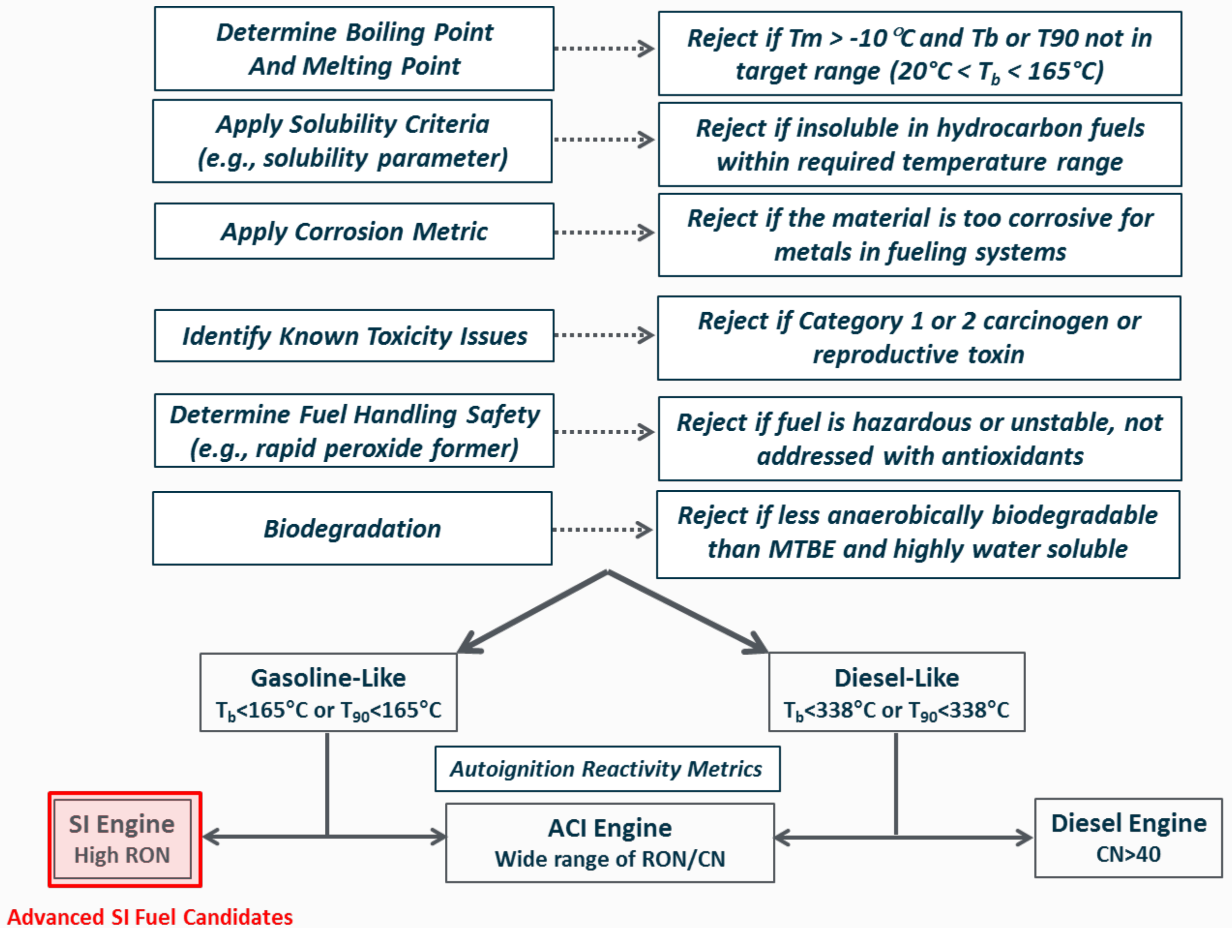
Tier 1

> 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



Fuel Property Database*

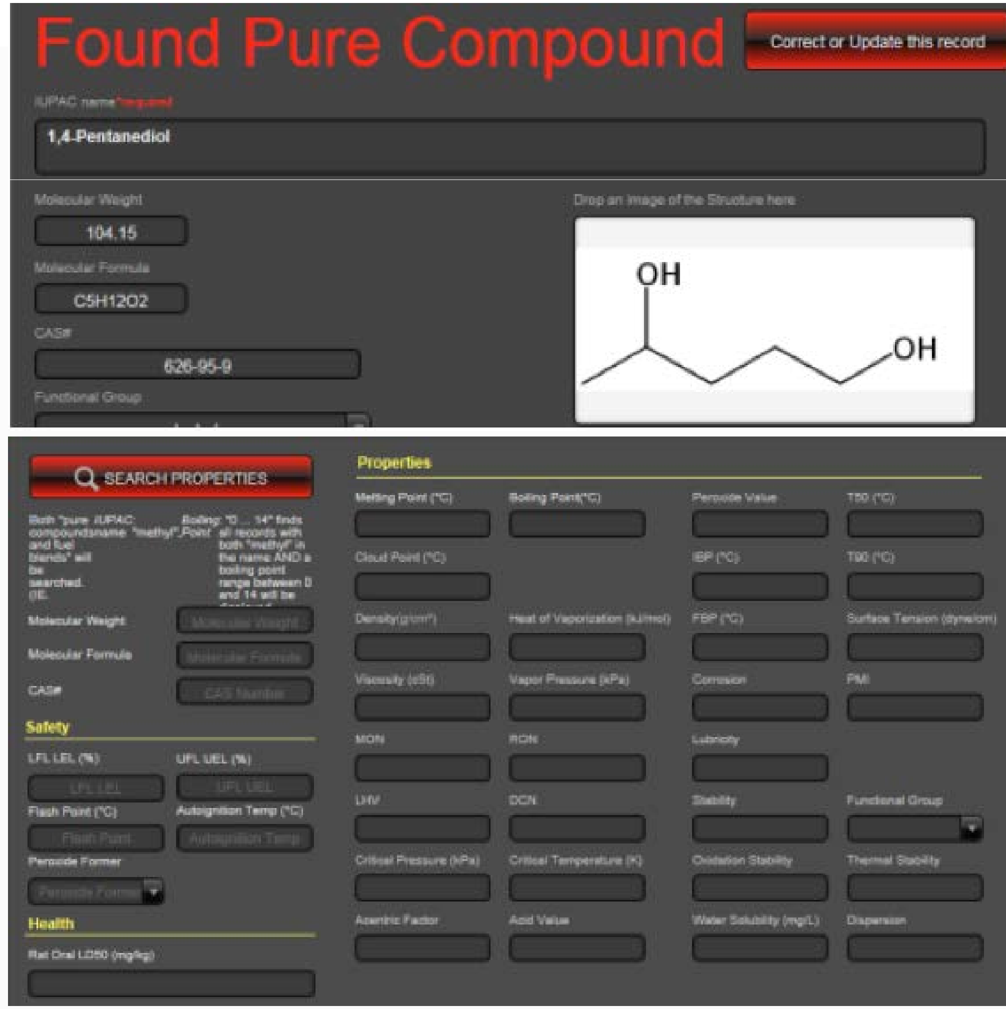
Tier 1

> 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

- Hydrocarbons
  - Normal paraffins
  - Iso-paraffins
  - Cycloparaffins
  - Olefins
  - Multi-ring aromatics
- Alcohols
- Furans
- Ethers
- Carbonyls
  - Ketones
  - Aldehydes
- Esters
  - Volatile fatty acid esters
  - Fatty esters
- Carboxylic Acids

YES →
- Normal paraffins
- Iso-paraffins
- Cycloparaffins
- Olefins
- Alcohols

YES FOR SOME →
- Aromatics
- Ketones
- Volatile fatty acid esters
- Furans
- Ethers

NO →
- Multi-ring aromatics
- Aldehydes
- Fatty esters
- Carboxylic acids

Tier 2 – blendstock evaluation

Tier 1	Tier 2
> 470 blendstocks	41 blendstocks
14 chemical families	10 chemical families
Identify broad range of potential hydrocarbon and oxygenated blendstocks	Measure blendstock properties
	Evaluate blendstock performance in BOBs at 10-30% blend levels
Utilize property information on blendstocks from literature or estimates to identify Tier 2 blendstocks	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

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

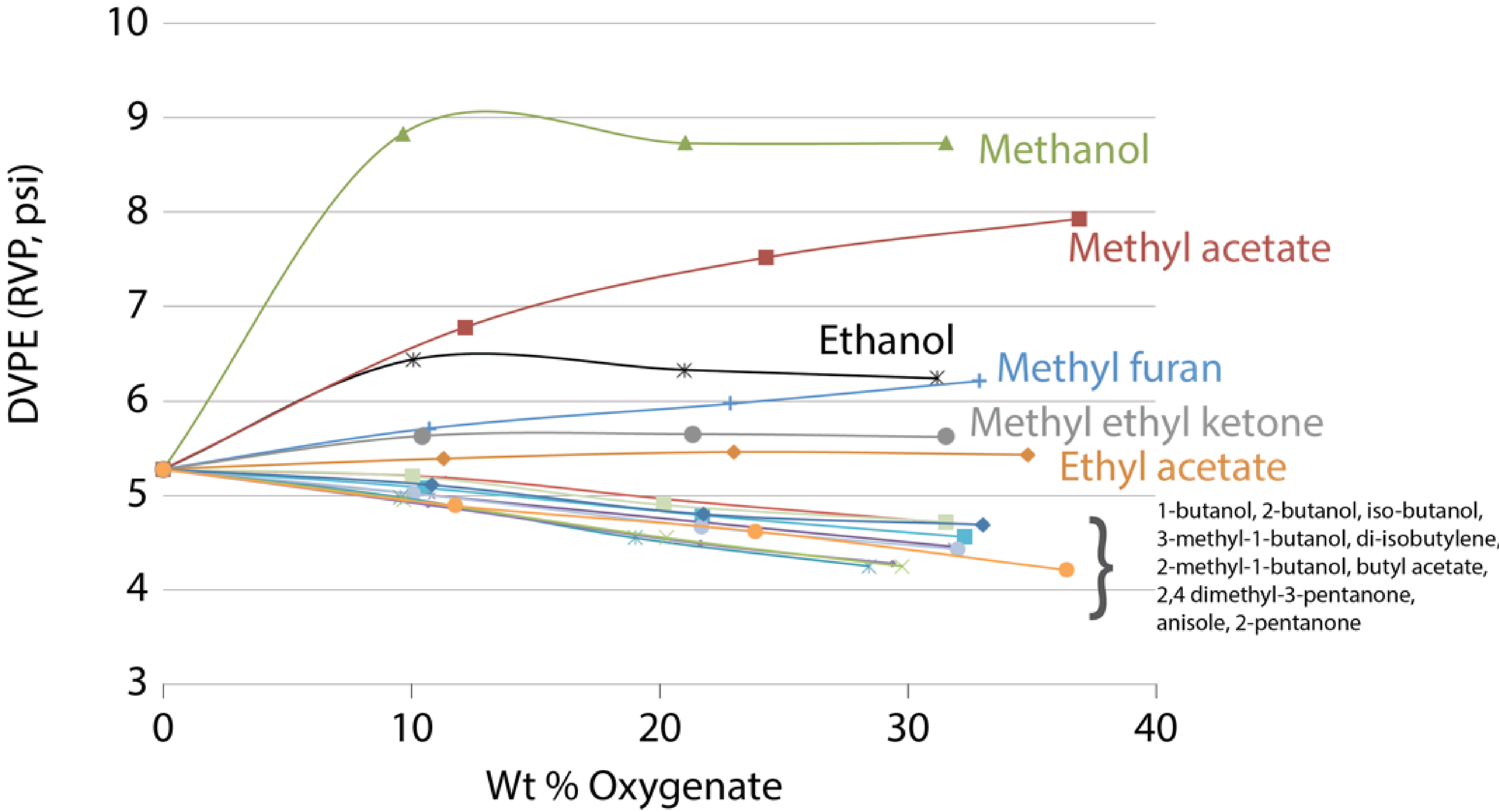
Furans	
33	2,5-Dimethylfuran/2-methylfuran

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

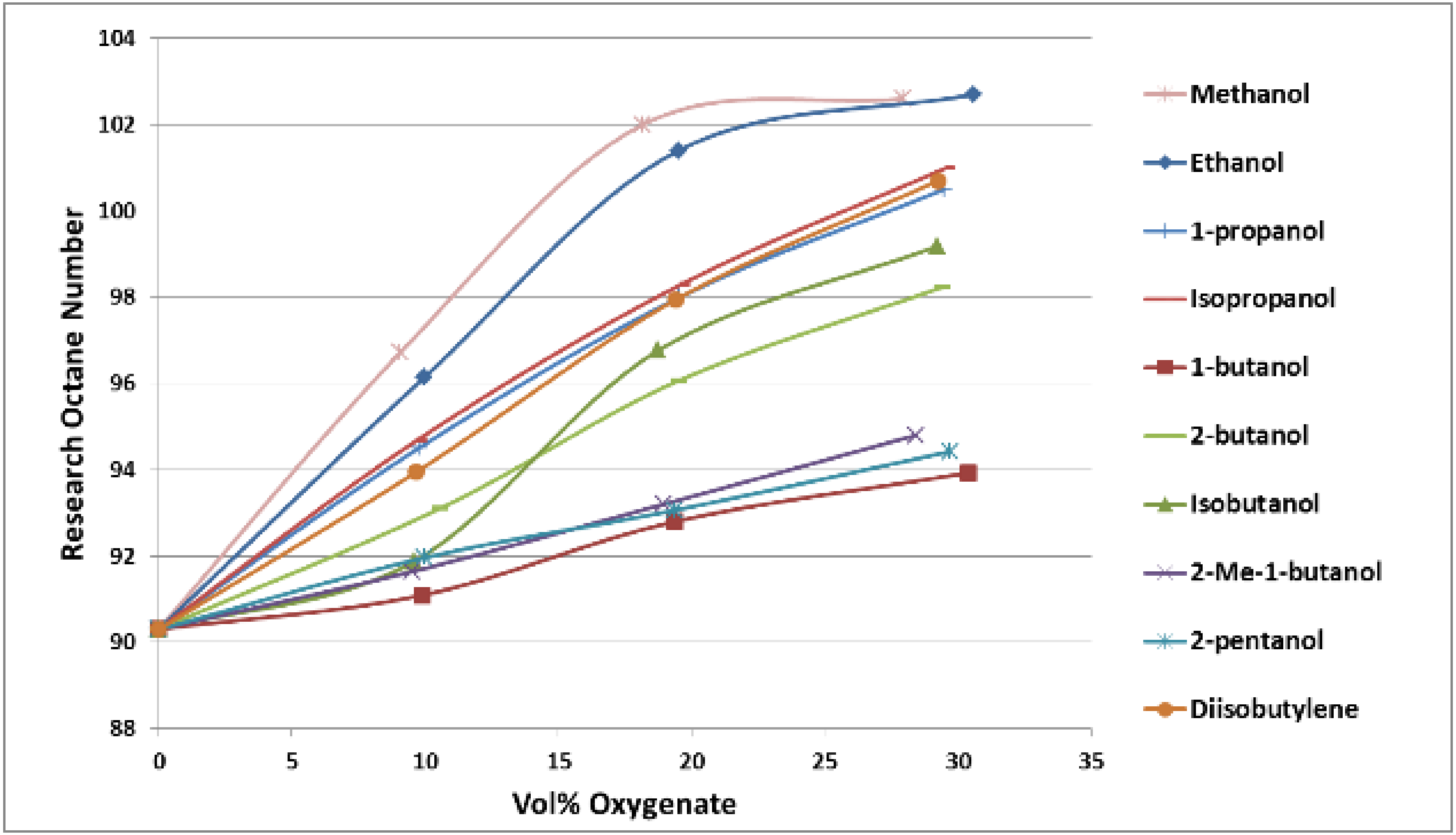
RVP data



Blending properties of blendstocks measured in 5.3 psi RVP RBOB

Large impact of methanol, methyl acetate on RVP present barriers to wide-spread use

Blending Octane Data



Categories for assessing blendstock viability

Technology Readiness	Environmental	Economics	Market
SOT - fuel production	Carbon efficiency	Target cost	Uncertainty
SOT - vehicle use	Target yield	Needed cost reduction	Regulatory requirements
Conversion TRL level	Life cycle GHG	Co-product economics	Geographic factors
Feedstock sensitivity	Life cycle water	Feedstock cost	Political factors
Process robustness	Life cycle FE use	Alternative high-value use	Vehicle compatibility
Feedstock quality			Infrastructure compatibility
# of viable pathways			

SOT = state of technology; TRL = technology readiness level; GHG = greenhouse gas; FE = fossil energy

- Twenty three metrics identified to assess feasibility of commercial introduction in 2025-2030 timeframe
- Technology readiness, environmental, and economic analyses restricted to bio-derived pathways (addresses gap in understanding)
- Market assessments apply to both petroleum- and bio-derived routes

Elastomer and plastic compatibility assessed

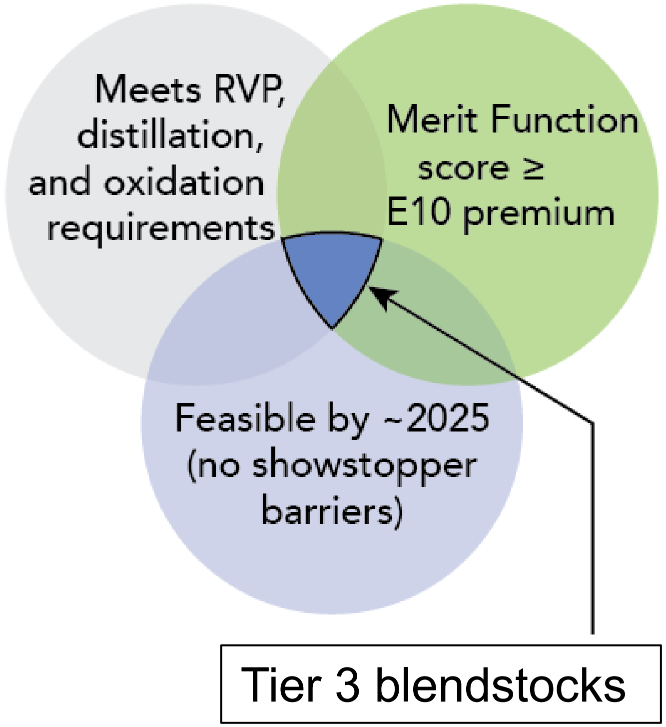
Promising Thrust 1 bio-blendstocks compared to gasoline and E10		Fluorocarbon			Silicone			Neoprene			Polyurethane			NBR			SBR		
		LBC	MRC	HBC	LBC	MRC	HBC	LBC	MRC	HBC	LBC	MRC	HBC	LBC	MRC	HBC	LBC	MRC	HBC
Alcohols	n-Propanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Propanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	1-Butanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Butanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Methylpropan-1-ol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Methyl-butanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Methyl-3-buten-2-ol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	2-Pentanol	C	C	C	I	I	C	C	I	C	C	C	C	I	C	C	I	C	C
	Ethanol	C	C	C	I	I	C	C	I	C	I	I	I	I	U	C	I	U	C
Alkanes	2,2,4 Trimethylpentane	C	C	C	I	I	C	C	I	C	C	C	C	U	C	C	U	C	C
Alkenes	Sabinene	C	C	C	I	I	I	C	U	U	C	C	C	U	I	I	U	I	I
Aromatics	1,3,5 Triethylbenzene	C	C	C	I	I	I	C	C	C	C	C	C	U	I	I	U	I	I
	1,3,5 Trimethylbenzene	C	C	C	I	I	I	C	C	C	C	C	C	U	I	I	U	I	I
Esters	Methyl acetate	C	U	U	I	I	I	C	I	I	C	C	U	U	U	C	I	I	C
	Ethyl acetate	C	U	U	I	I	I	C	I	I	C	C	U	U	U	C	I	I	C
	Pentanoic acid	C	I	C	I	I	C	C	I	C	C	U	C	I	C	C	I	C	C
	Propionic acid	C	C	C	I	I	U	C	U	C	C	C	C	I	C	C	I	C	C
	Methylbutanoate	C	C	C	I	I	I	C	I	U	C	C	C	U	I	U	I	U	U
	Butyric acid	C	C	C	I	I	I	C	I	C	C	C	C	U	U	C	U	U	C
	Ethyl propionate	C	U	I	I	I	I	C	U	I	C	C	U	U	I	U	U	I	U
	Isopropyl acetate	C	C	C	I	I	I	C	I	I	C	C	C	U	U	C	U	U	C
	Butyl acetate	C	C	C	I	I	I	C	I	I	C	C	C	U	U	U	I	I	U
	Isoamyl acetate	C	C	C	I	I	I	C	I	I	C	C	C	U	U	U	I	I	U
Ethers	Methoxybenzene	C	C	C	I	I	I	C	I	I	C	C	U	U	I	I	I	I	I
	2-Methylfuran	C	C	C	I	I	I	C	I	I	C	C	C	U	I	I	I	I	U
	2,5-Dimethylfuran	C	C	C	I	I	I	C	I	I	C	I	I	U	I	I	I	I	I
	Furanic mixture (60% dimethyl furan/40%2-methylfuran	C	C	C	I	I	I	C	I	I	C	I	I	U	I	I	I	I	I
Ketones	2-Butanone	C	C	U	I	I	I	C	U	U	C	C	C	U	U	C	I	I	C
	2-Pentanone	C	U	I	I	I	I	C	U	U	C	C	U	U	U	U	I	I	U
	3-Pentanone	C	U	I	I	I	I	C	I	I	C	C	I	U	I	C	I	I	C
	2-Propanone	C	I	I	I	I	I	C	I	C	C	U	I	U	I	C	I	I	C
	Cyclopentanone	C	I	C	I	I	I	C	I	C	C	I	I	U	I	C	I	I	C
	Ethyl 2-methylpropanoate	C	C	U	I	I	I	C	I	I	C	C	C	U	I	C	I	I	C
Gasoline Surrogate (dodecane)		C			I			C			C			C			I		
E10 surrogate (10% ethanol in dodecane)		C			I			C			C			C			C		

Key

LBC	low blend content (~10-30%)	C	Likely compatible
MRC	mid range blend content (~30-70%)	I	Likely incompatible
HBC	high blend content (~70-100)	U	Uncertain

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
   - Candidates must have viable path to potential market introduction by ~2025-2030

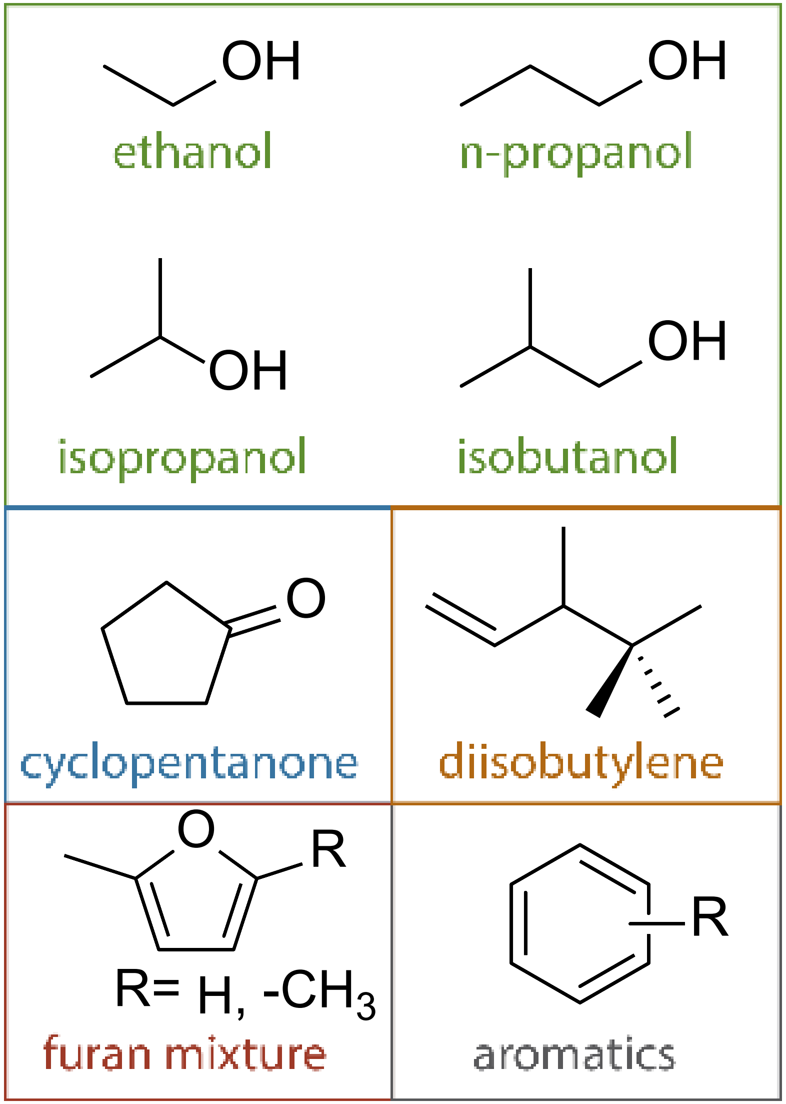


Tier 2 → 3 transition allows focused effort on blendstocks with greatest potential to meet Co-Optima goals

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

Tier 3 blendstocks

- Eight representative blendstocks identified for prioritized R&D in Tier 3
  - No further downselects are planned
- Next steps include:
  - Refine property measurements
  - Improve blending models
  - Engine tests to confirm performance
  - Emissions control experiments to assess impact
  - Confirm potential to meet FE targets
  - More detailed life cycle and techno-economic analyses
  - Utilize final validated merit function as technical basis for new fuel-property-based specification



Summary and 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 and evaluations of eight Tier 3 representative candidates to
  - Provide critical information to industry/regulatory stakeholders
  - Provide foundation for development of fuel specification
  - Assess candidates for potential follow-on scale-up studies (outside Co-Optima)
- Expand LD efforts to include multi-mode SI-ACI combustion
- Expand multi-team ACI research for MD- and HD applications
- Develop approach (e.g., identification of critical fuel properties, merit function, fuel screening, simulation, etc.) for advanced gasoline multi-mode and ACI combustion platforms
- Continued strong engagement with stakeholders to help focus R&D on options that provide “wins” for broad range of stakeholders

Backup Slides

2017 BETO Peer Review Presentations

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BIOENERGY

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

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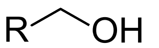
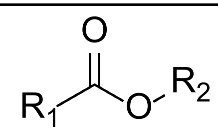
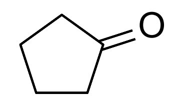
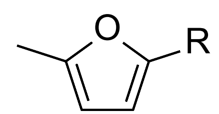
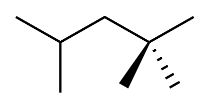
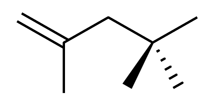
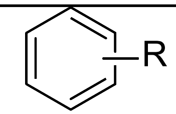
The Bioenergy Technologies Office hosted its 2017 Project Peer Review on March 6-9, 2017, in Denver, Colorado. The presentations from the Co-Optimization of Fuels and Engines sessions are available to view and download below. For detailed session descriptions and presentation titles, view the 2017 Project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

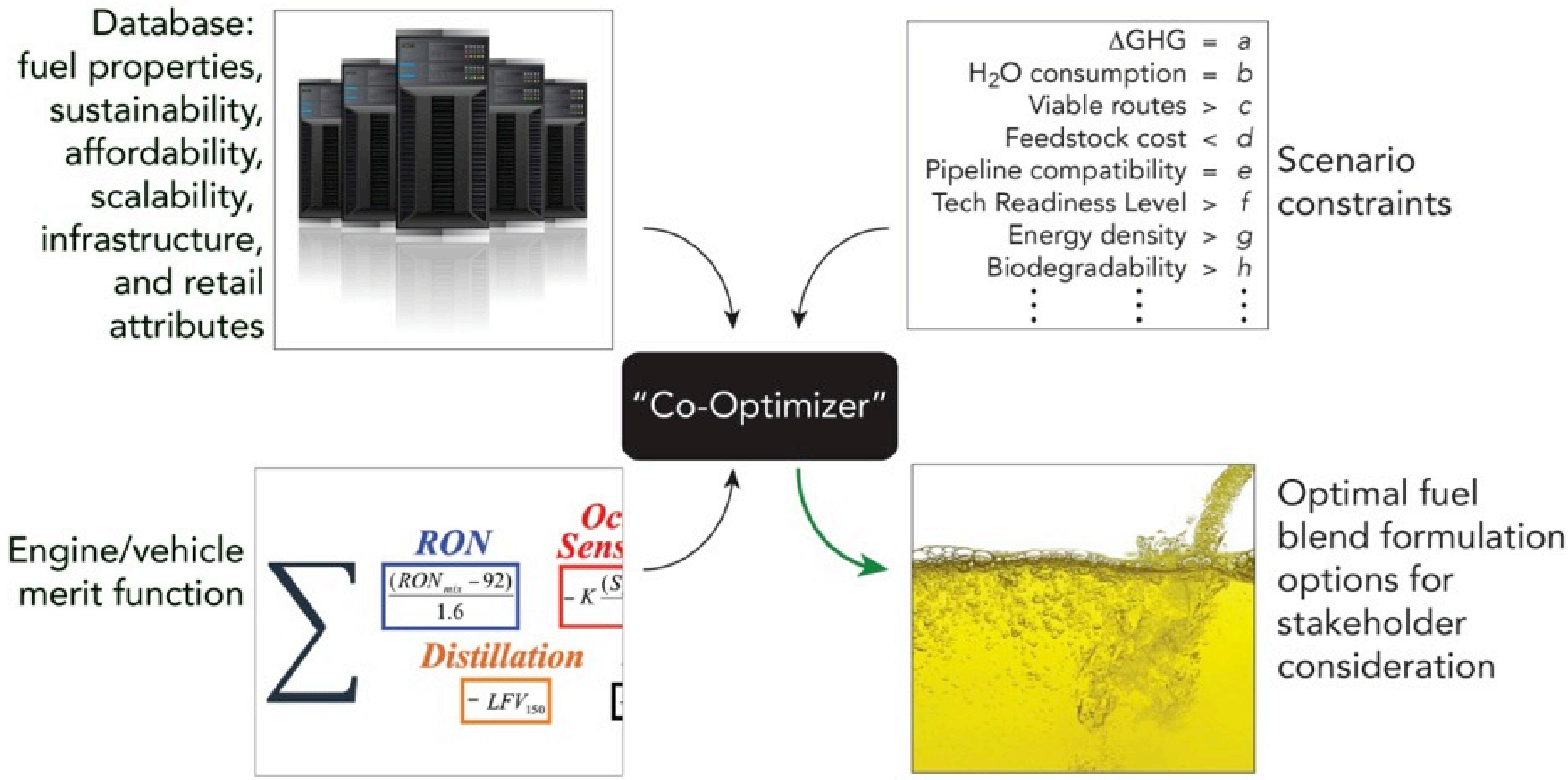
Eight representative Tier 3 blendstocks

Alcohols – high RON, S, HOV, higher alcohols require branching (Tier 3: C2-C4 with branching)	
Esters – High RON/MON, low S and antagonistic blending (Tier 3: stop)	
Ketones – High RON, branching needed for S; need to assess compatibility (Tier 3: further study on cyclopentanone)	
Furans – High RON and S; need to explore oxidative stability (Tier 3: further study on furans)	
n-/i-Alkanes – Require branching for octane, limited S (Tier 3: stop, however may consider alkylates in BOB)	
Alkenes – Improves RON and S, high LHV (Tier 3: evaluate representative large, 8 carbon, alkenes	
Aromatics – High RON and S (Tier 3: evaluate bioreformate)	

Main elements of approach

- Identify key fuel properties that impact efficiency for advanced SI and CI combustion approaches
  – Utilize "efficiency merit function" to identify most important property impacts
  – Utilize final validated merit function as technical basis for fuel property specification
- Apply tiered approach to identify blendstock options that provide key fuel properties
  – Identify barriers to widespread commercial introduction
  – Focus on options with viable routes to near-term commercial use (petroleum- or bio-based)
  – Identify blendstocks that provide value when produced from biomass
- Identify ways to co-optimize, i.e., identify options that provide "wins" for broad range of stakeholders

Co-Optimizer – Approach and Tool



The Co-Optimizer computational tool will identify fuel formulations that meet commercial fuel specifications and maximize engine efficiency, subject to various constraints

Efforts underway to clarify value propositions for all major stakeholder groups (including consumers)

Goal is to identifying deployment scenarios with maximum market pull for all stake-holder groups (a "win" for all)

Remaining Challenges and Barriers

- Ensuring research pathways (e.g., boosted SI, ACI, etc.) have value for all stakeholders – this is critical for ensuring impact of this initiative on the introduction of better fuels and vehicles
- Further understanding of interdependencies of fuel properties and finalization of the merit function for advanced gasoline SI
- Understanding critical fuel properties for multimode SI-ACI combustion
- Identifying fuel properties critical for enabling higher engine system efficiency for ACI combustion
- Selecting high potential ACI combustion modes for the formation of multi-team research plans
- Maintaining strong stakeholder engagement

Collaboration/Coordination with Other Institutions

- Collaboration across nine national laboratories and two DOE offices
- Eight universities awarded up to $7M in FY17 FOA
  - Intent is to fully integrate university and national lab efforts
  - Kickoff meeting held April 28, 2017
  - Each team assigned a national lab “mentor” to facilitate integration and coordination
- Stakeholders (129 individuals from 77 organizations)
  - External advisory board (advising national labs, not DOE)
  - Monthly telecons with technical and programmatic updates
  - One-on-one meetings and conference presentations
  - Listening Days (three thus far)

Proposed Future Research

- Refine merit function development and establish technical basis for advanced gasoline fuel specification for boosted SI by end of FY18
- Initiate assessments and evaluations of eight Tier 3 representative candidates to
  - Provide critical information to industry/regulatory stakeholders
  - Provide foundation for development of fuel specification
  - Assess candidates for potential follow-on scale-up studies (outside Co-Optima)
- Expand advanced gasoline research to include multi-mode SI-ACI combustion
- Initiate multi-team ACI research for MD- and HD applications
- Develop approach (e.g., identification of critical fuel properties, merit function, fuel screening, simulation, etc.) for advanced gasoline multi-mode and ACI combustion platforms
- Continued strong engagement with stakeholders

Much more detail will be presented in subsequent presentations

Summary

Relevance

- Better integration of fuels and engines research critical to accelerating progress towards economic development, energy security, and emissions goals

Approach

- Focused on identifying fuel properties that optimize engine performance, independent of composition, allowing the market to define the best means to blend and provide these fuels
- Leverages expertise and facilities from nine national laboratories and two DOE offices

Technical Accomplishments

- Major accomplishments span development of merit function, fuel database, new insight into fuel property impacts on engine efficiency, etc.
- Many additional accomplishments will be discussed in detail in subsequent presentations

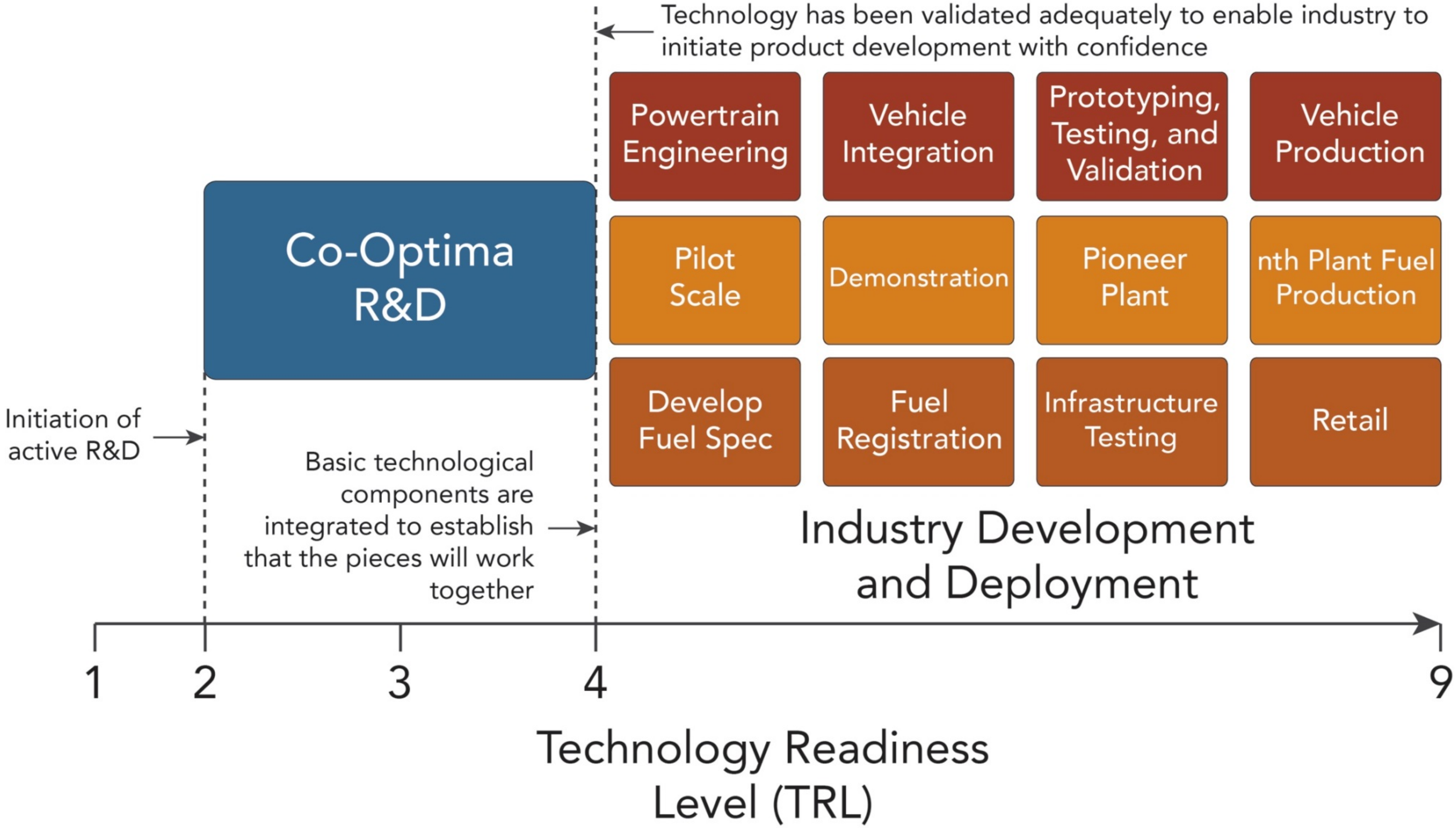
Proposed Future Research

- Complete merit function development and establish fuel specification for boosted SI
- Expand advanced gasoline research to include multi-mode SI-ACI combustion
- Initiate more focused ACI research and approach for medium- and heavy-duty

Collaborations

- Strong industry engagement including industry-led external advisory board, monthly stakeholder phone calls, and annual stakeholder meeting
- Collaboration across nine national laboratories, two DOE office, and thirteen universities

Engagement with Industry



Partners – University Teams

1. Yale Univ./Penn State Univ.
   Measure sooting tendencies of various biofuels and develop emission indices
2. Univ. Michigan
   Engine combustion model simulating combustion duration, flame speed, and pressure development
3. Louisiana State Univ./Texas A&M/Univ. Connecticut
   Models and metrics for predicted engine performance
4. Univ. Alabama
   Combustion properties of biofuels and blends under realistic (ACI) engine conditions
5. Cornell University/UC San Diego
   Combustion characteristics of several diesel/biofuel blends
6. MIT/Univ. Central Florida
   Detailed kinetic models for several biofuels
7. Univ. Michigan-Dearborn/Oakland Univ.
   Miniature ignition screening rapid compression machine
8. Univ. Central Florida
   Measure and evaluate fuel spray atomization, flame topology, volatility, viscosity, soot/coking, and compatibility

Co-Optima Organization

Board of Directors
(Labs and DOE)
Approve direction and changes in focus

Steering Committee
POC for each lab, communications, IP

Operations
Project management, project integration, and strategic consulting

Leadership Team
(Labs and DOE)

Establish vision, define strategy, integrate work plan, oversee execution, evaluate performance, engage stake holders, and team build

External Advisory Board
Advise on technology and direction, provide recommendations, bridge to stakeholders

Technical Team Leads
Plan projects, evaluate team performance and gaps, report monthly highlights and quarterly progress, communicate across teams to minimize silos

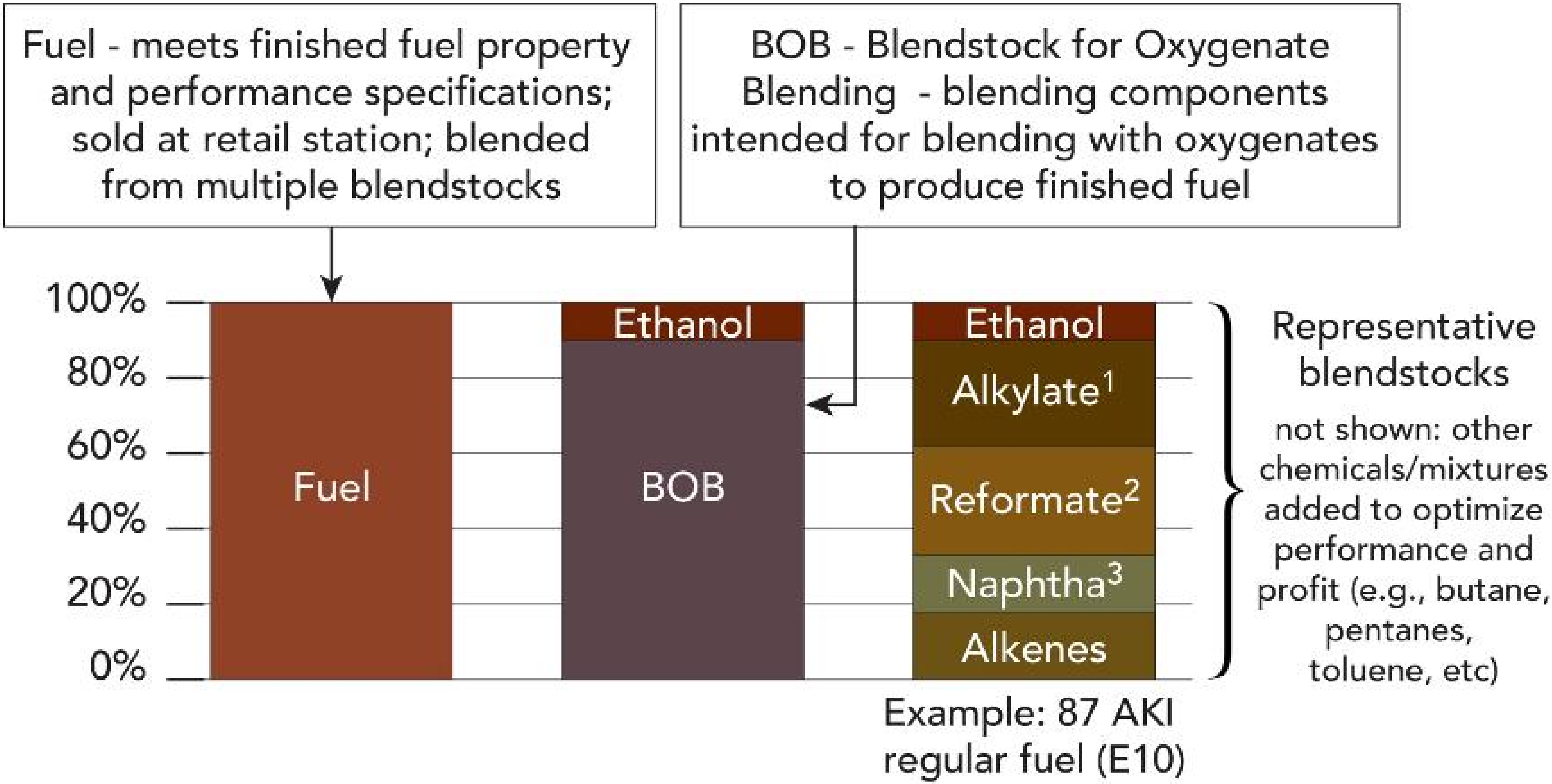
Relevance

- Internal combustion engines will dominate the fleet for decades and their efficiency can be increased significantly
- Research into better integration of fuels and engines is critical to accelerating progress towards economic development, energy security, and emissions goals
- Improved understanding in several areas is critical for progress:
    - Fuel chemistry – property relationships
    - How to measure and predict fuel properties
    - The impact of fuel properties on engine performance
- Relevant to LD SI, MD/HD diesel, and ACI combustion strategies
- Addresses VTO program plan knowledge gaps surrounding advanced combustion engine regimes and predicting the impact of fuel properties

Overall Co-Optima Objectives

- Identify engine parameters and fuel properties that can significantly increase fuel economy across light, medium, and heavy duty fleets
  - Focus is on precompetitive, early TRL research
  - We are not looking to define or recommend commercial solutions
- Develop technical knowledge needed for new fuel specifications
- Conduct comprehensive and consistent survey of blendstock candidates to identify broad range of options that can be blended into petroleum base stocks and yield target values of key properties
- Demonstrate blendstock candidates that can be produced from renewable domestic feedstocks that are affordable, scalable, sustainable, and compatible
- Identify implications to the refueling infrastructure for the various blendstock options
- Develop tools that allow us to do the work faster and more efficiently
- Identify options that provide "wins" for broad range of stakeholders

Blendstock vs Fuel



1) primarily comprised of iso-paraffins; 2) primarily aromatics; 3) primarily paraffins (n-, iso-, cyclo)

Partners – 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)

- EAB advises National Lab Leadership Team
- Participants represent industry perspectives, not individual companies
- Entire board meets twice per year; smaller groups meet on targeted issues

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

Univ. Michigan - Dearborn

Use a miniature ignition screening RCM to study ignition properties and 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 Florida

Generate fuel characterization data related to fuel spray atomization, flame topology, etc, and compatibility for prioritized fuels