Co-Optimization of
Fuels & Engines

DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Co-Optima Overview

Co-Optima Review Session
March 7, 2019

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Pacific Northwest National Laboratory


better fuels | better vehicles | sooner

1 – Project Overview
Improving biofuel value through co-optimization

Goal

Identify low carbon fuel-engine combinations that increase fuel economy by 35% (light duty) or 4% (heavy duty) over a 2015 baseline, with reduced emissions

Outcome

Improved definition of the critical fuel properties that maximize engine efficiency, the bio-blendstocks that provide target values of these fuel properties, and the potential impacts of adoption in reducing harmful emissions and providing environmental and economic benefits

Relevance

Provides foundational knowledge to stakeholders to improve the value proposition for biofuels

"Better fuels, better vehicles, sooner"

Engine R&D

Fuel R&D

Quad Chart Overview

Timeline

- Start: FY2016
- Merit Review Cycle: FY2019 to FY2021
- 12% complete of review cycle

	Total Budget Pre-FY17	FY 17 Budget	FY 18 Budget	Total Planned Funding (FY 19-21)
BETO Funded	$14,000	$12,000	$12,600	$36,000
VTO Funded	$12,000	$12,500	$12,500	$36,000

Partner Labs: ANL, INL, LANL, LBNL, LLNL, NREL, ORNL, PNNL, SNL

Barriers Addressed

- ADO-E. Co-Development of Fuels & Engines
- At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts

Objective

Advance the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals

End of Project Goal

Identify low carbon fuel-engine combinations that increase fuel economy by 35% (light duty) or 4% (heavy duty) over a 2015 baseline, with reduced emissions

Budget by Lab (k$)*

Lab	Total Budget Pre FY17	FY 17 Budget	FY 18 Budget	FY19-end Budget
ANL	$840	$900	$1,000	$2,970
INL	$1,300	$540	$305	$240
LANL	$700	$710	$784	$1,875
LBNL	$1,100	$860	$1,030	$2,100
NREL	$4,100	$4,200	$4,784	$13,680
ORNL	$900	$670	$816	$2,730
PNNL	$3,100	$2,400	$2,110	$7,020
SNL	$2,300	$1,600	$1,769	$5,385
Total	$14,000	$12,000	$12,598	$36,000

* Only funding from BETO shown

2 – Approach (Management)

Goals and outcomes target national impact

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

Diversify resource base

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

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

Cross-cutting goals

Stimulate domestic economy

Add new bio-economy jobs

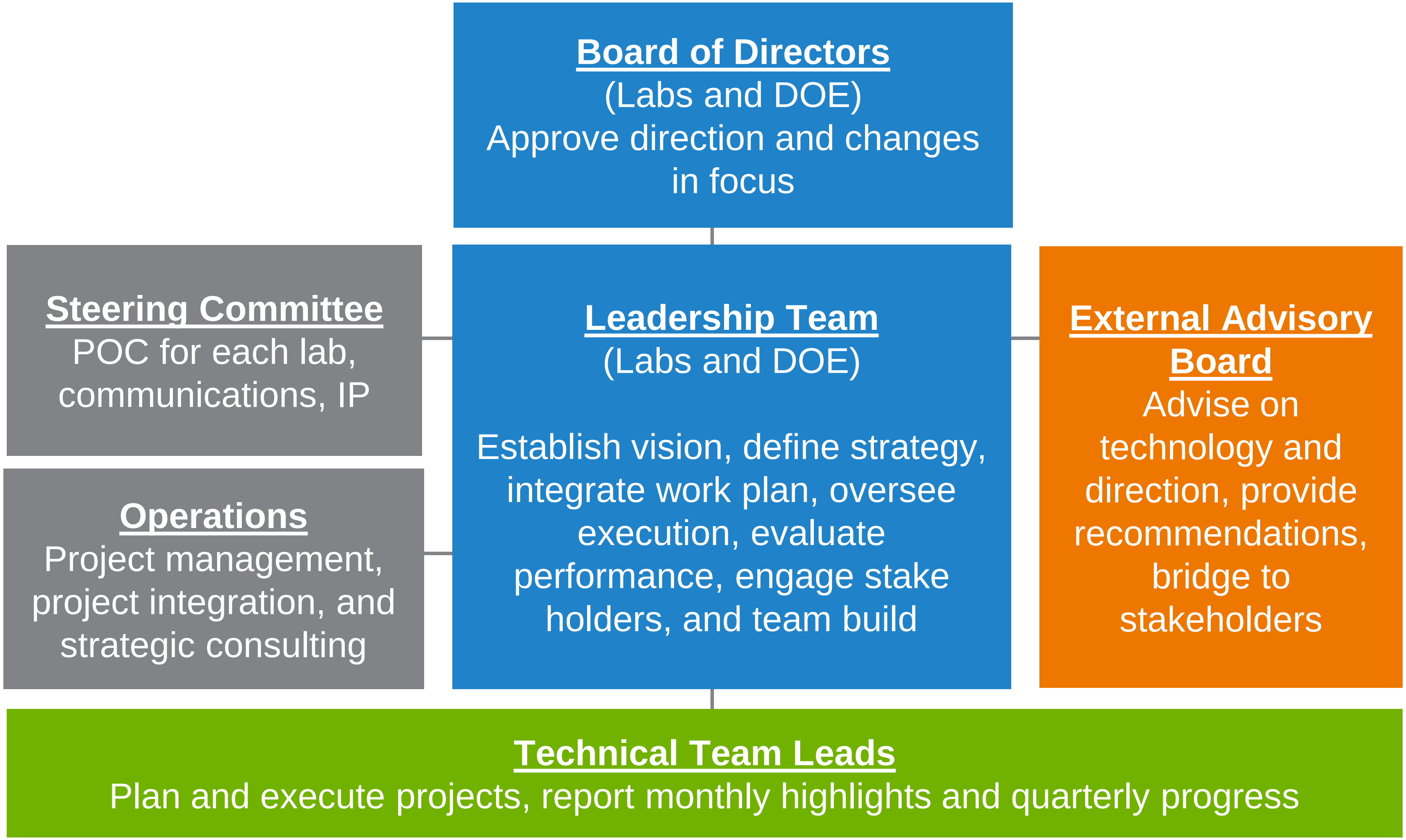
Provide clean-energy options

* 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.

2 - Approach (Management)

Organized to ensure coordination



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 and execute projects, report monthly highlights and quarterly progress

A formal "Roles and Responsibilities" document has been developed that is regularly updated and available on the Co-Optima team SharePoint site

Extended Leadership Team = Leadership Team, DOE, Steering Committee, Team Leads

2 – Approach (Management)

Leadership draws on DOE and Labs

Board of Directors

Senior leadership (EERE and labs)

DOE

- Michael Berube (EERE)
- Jonathan Male (BETO)
- Dave Howell (VTO)

Labs (Assoc. Lab Directors)

- Johney Green (NREL)
- Moe Khaleel (ORNL)
- Jud Virden (PNNL)
- Dori Ellis (SNL)

Leadership Team

Leaders from VTO, BETO and labs

DOE

- Alicia Lindauer (BETO)
- Kevin Stork (VTO)

Labs

- Robert Wagner, Lead (ORNL)
- Dan Gaspar (PNNL)
- Bob McCormick (NREL)
- Chris Moen (SNL)

2 – Approach (Management)
EAB includes autos, (bio)fuels, regulatory experts

USCAR
David Brooks

American Petroleum Institute
Scott Mason

Fuels Institute
John Eichberger

Truck & Engine Manufacturers Assn
Roger Gault

LanzaTech
Laurel Harmon

Flint Hills Resources
Chris Pritchard

EPA
Paul Machiele

California 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)

- External Advisory Board advises National Lab Leadership Team
- Participants represent industry perspectives, not individual companies
- Entire board meets twice per year, with quarterly teleconferences to keep them up to date

2 – Approach (Management)

Technical team leads and roles clearly defined

HPF

Anthe George (SNL)
Derek Vardon (NREL)

ASSERT

Jennifer Dunn (ANL)
Mary Biddy (NREL)

TK

Matt McNenly (LLNL)
Sibendu Som (ANL)
Ray Grout (NREL)

AED

Magnus Sjoberg (SNL)
Josh Pihl (ORNL)

FP

Jim Szybist (ORNL)
Gina Fioroni (NREL)

Roles and Responsibilities: Plan and execute projects, report monthly highlights and quarterly progress

2 – Approach (Management)

Outreach provides 2-way communication

Stakeholder “Listening Days”

Stakeholder visits

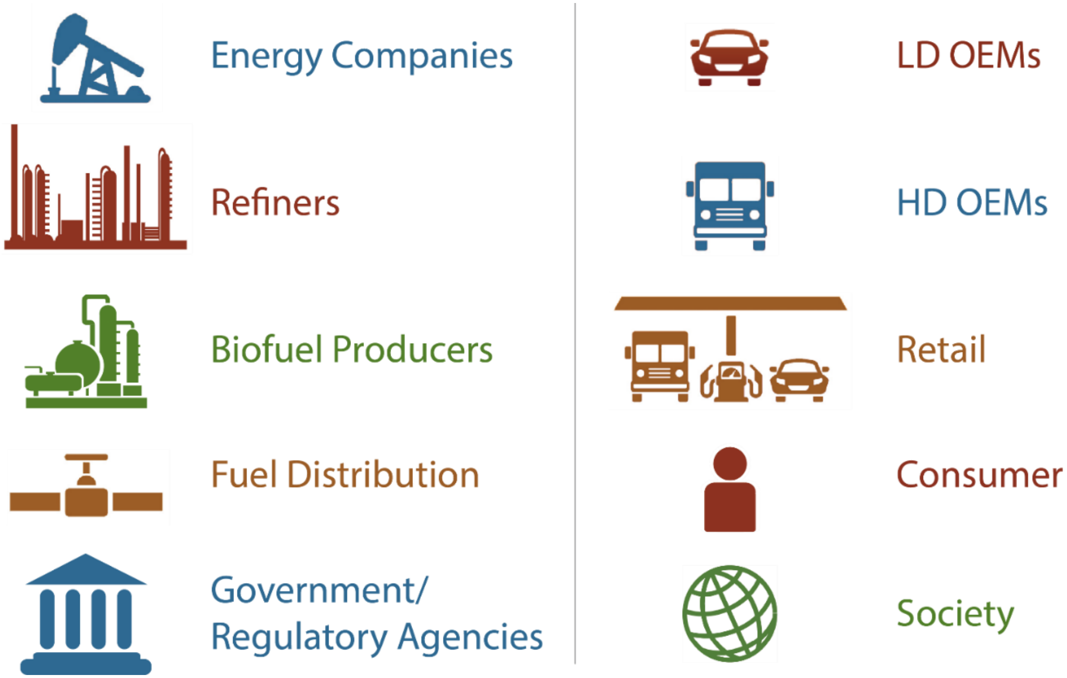
- Individual visits to OEMs, fuel providers, retail organizations, biofuel companies, etc.
- More than 60

Interactive forums through technical societies

Monthly webinars

- 145 individuals
- 86 organizations

VTO Annual Merit Review and BETO Peer Review



Energy Companies

Refiners

Biofuel Producers

Fuel Distribution

Government/ Regulatory Agencies

LD OEMs

HD OEMs

Retail

Consumer

Society

2 – Approach (Management)
Project plan and program management

A project plan is developed annually for this consortium project to organize the work across the Labs

A full-time project manager is utilized to ensure task coordination and milestone completion

Co-Optimization of Fuels & Engines

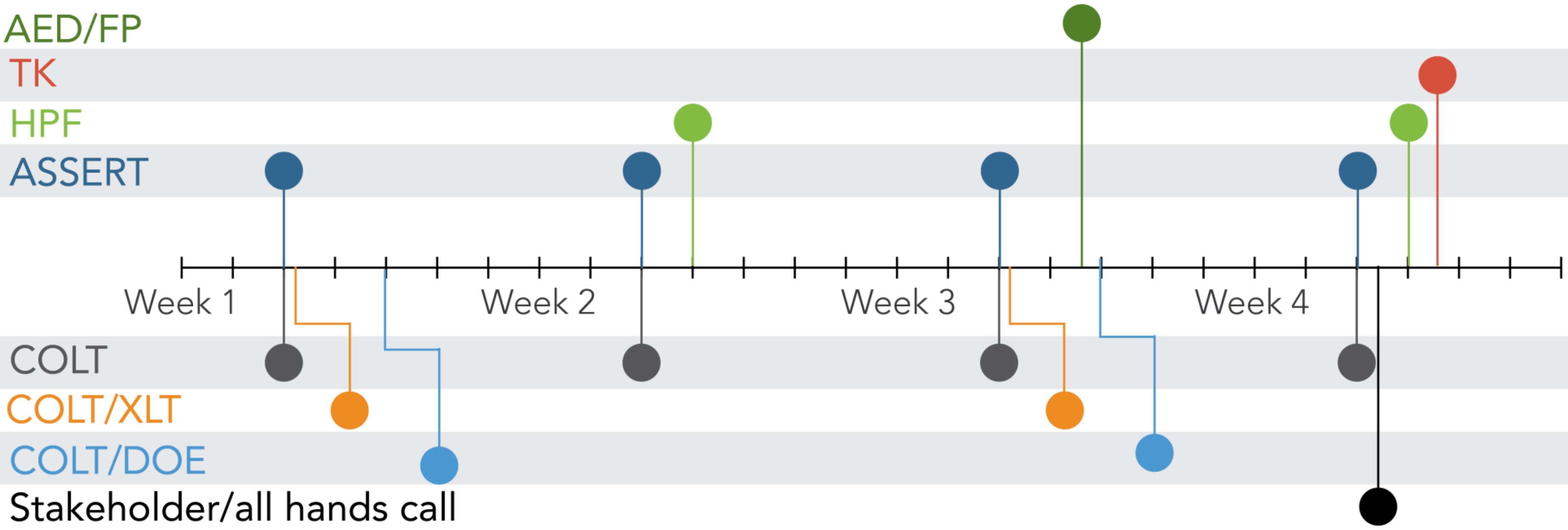
FY17 Project Plan

Project Task/Team Detail

2 – Approach (Management)

Communication and coordination are essential

Co-Optima regularly scheduled meetings

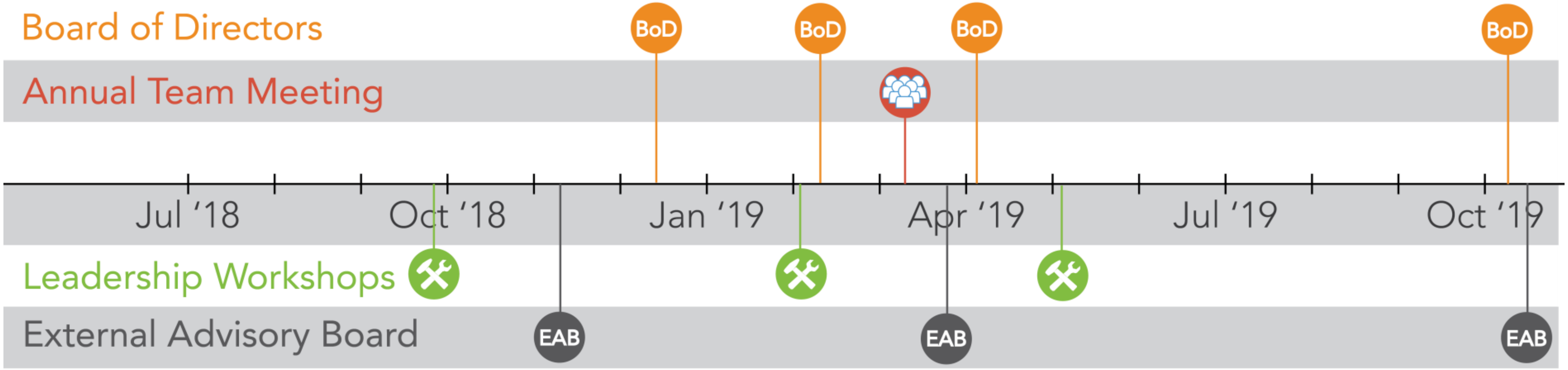


Regular team meetings have cross-team participation

AED/FP: Advanced Engine Development/Fuel Properties; TK: Modeling and Simulation Toolkit; HPF: High Performance Fuels; ASSERT: Analysis of Sustainability, Scale, Economics, Risk, and Trade; COLT: Co-Optima Leadership Team; XLT: Extended Leadership Team (COLT, DOE, Team Leads, Steering Committee)

2 – Approach (Management)
Active engagement and stewardship

Co-Optima major events



2 – Approach (Technical)

Parallel projects address short and longer terms

Light-Duty

Boosted SI

Higher efficiency via downsizing

Near-term

(Boosted SI)

Multi-mode SI/ACI

Even higher efficiency over drive cycle

Mid-term

(MM)

Medium/Heavy-Duty

Mixing Controlled

Improved engine emissions

Near-term

(MCCI)

Kinetically Controlled

Highest efficiency and emissions performance

Longer-term

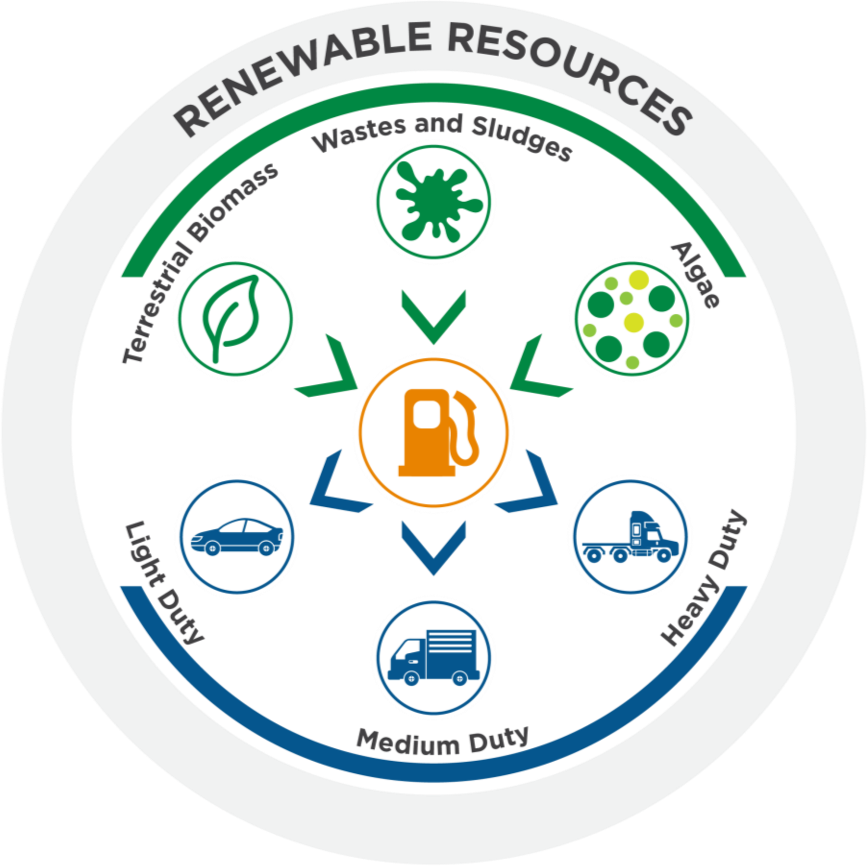
(KC)

2 – Approach (Technical)

Co-Optima is fuel property-based

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

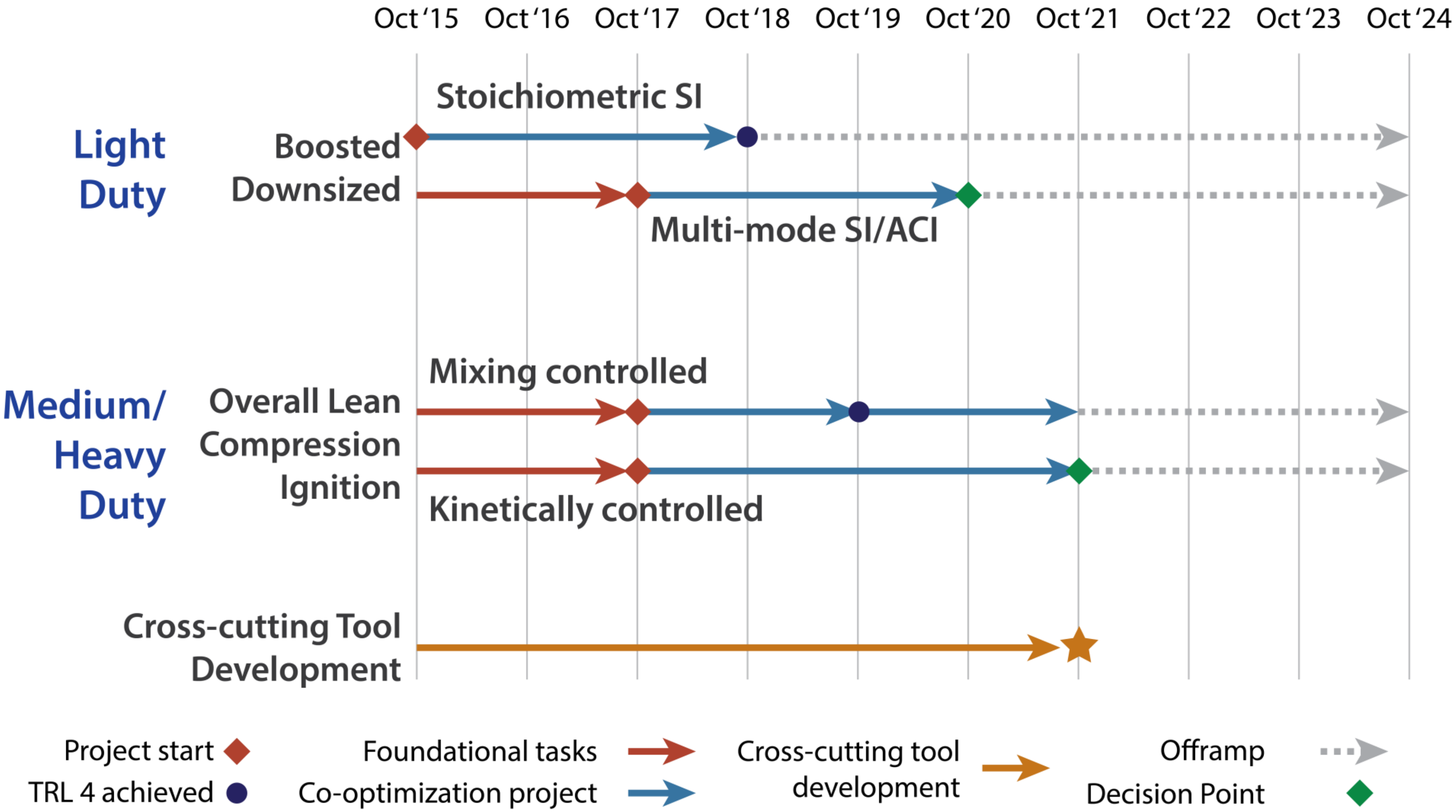


2 – Approach (Technical)
Key Co-Optima constraints define search space

- Focusing only on liquid fuels
- Identify blendstocks to blend into petroleum base fuel
- Considering only non-food-based biofuel feedstocks
- Assessing well-to-wheels impacts for biofuel options (GHG, water, economics,…)
- Evaluating impact of hybridization, but focused on internal combustion component
- Provide data, tools, and knowledge to stakeholders – objective is not to “pick winners”

2 – Approach (Technical)

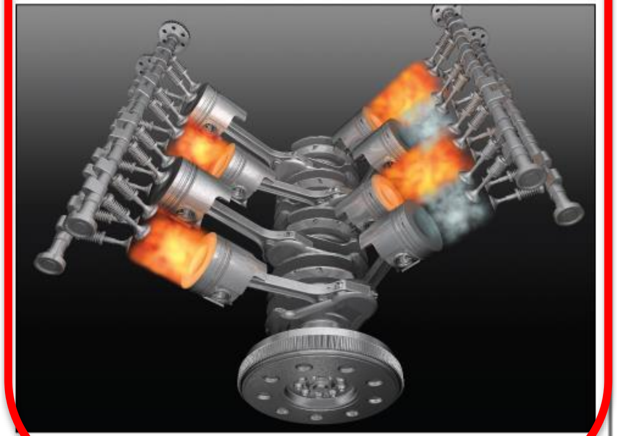
R&D staged for near & long-term challenges



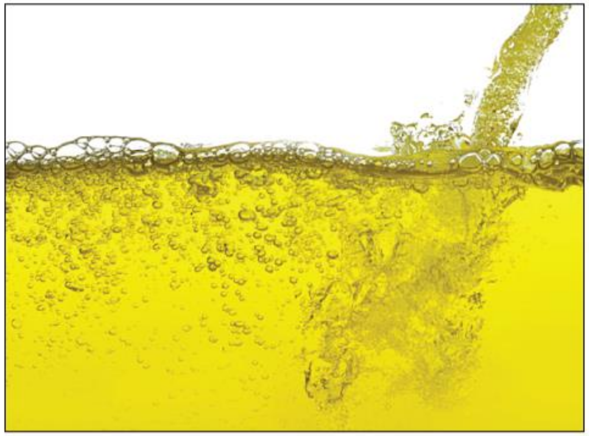
2 – Approach (Technical)

Foundational technical questions frame approach

What fuels do engines *really* want?



What fuel options work best?



What will work in the real world?

2 – Approach (Technical)

Engine R&D determines critical fuel properties

Light Duty Boosted SI merit function

$$\text{Merit (efficiency)} = \overbrace{\overset{\text{RON}}{\boxed{\alpha \cdot f(\text{RON})}} + \overset{\text{Octane Sensitivity}}{\boxed{\beta \cdot f(K, S)}}}^{\text{Octane Index (Knock)}} + \overbrace{\overset{\text{Heat of Vaporization}}{\boxed{\gamma \cdot f(\text{HOV})}}}^{\text{Charge Cooling}}$$

$$+ \underbrace{\underset{\text{Flame Speed}}{\boxed{\varepsilon \cdot f(\text{LFS})}}}_{\text{Burn Rate/ Dilution Tolerance}} + \underbrace{\underset{\text{PM Emissions}}{\boxed{\zeta \cdot f(\text{PMI})}} + \underset{\text{Catalyst Light-off Temp (cold start)}}{\boxed{\eta \cdot f(T_{c,90,conv})}}}_{\text{Emissions Penalties}}$$

AED FP

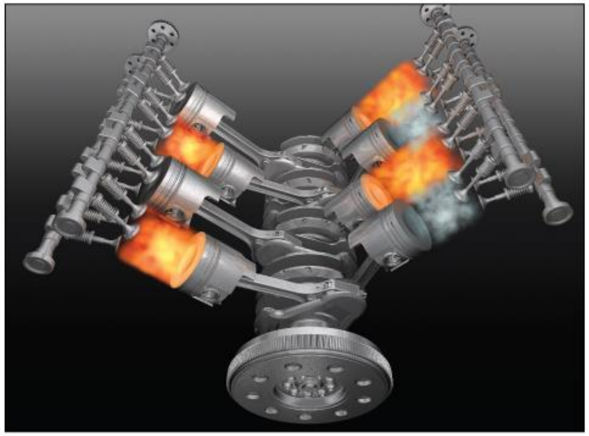
Medium/Heavy Duty MCCI (Diesel) merit table

Tier Criteria	Greatly Exceeds	Exceeds Criteria	Meets Criteria	Barriers Exist
Cetane	> 50	46 to 50	40 to 45	< 40
LHV (MJ/kg)	> 40	31 to 40	25 to 30	< 25
Flash Pt (°C)	> 70	61 to 70	52 to 60	< 52
Melting Pt (°C)	< -50	-50 to -26	-25 to 0	> 0
Water Sol (mg/L)	< 5	5 to 501	500 to 1000	> 1000
YSI	< 50	50 to 151	150 to 200	> 200

AED FP

2 – Approach (Technical)
BETO supports biofuel R&D and analysis

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

2 – Approach (Technical)

R&D and analysis develop options and identify impacts

Following presentations detail efforts in 4 key areas:

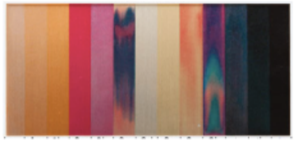
- Bio-blendstock structure-property relationships and property prediction tools
- Bio-blendstock generation
- Bio-blendstock fuel property measurements and characterization
- Techno-economic, life-cycle, infrastructure impacts and other analyses

2 – Approach (Technical)

Blendstock evaluation integrates disciplines

Rigorous Screening

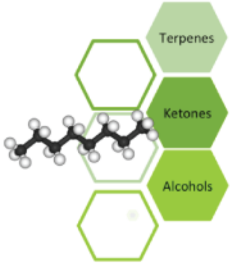
Rapidly identify viable candidates



Blendstock Evaluation

Measure properties

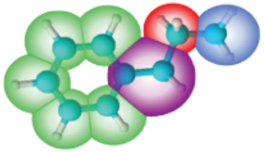
Populate database

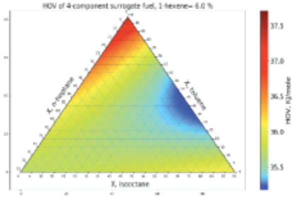


Generate Insight

Develop blending models

Correlate properties to molecular structure

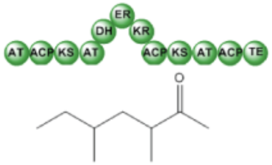




Establish Bio Pathways

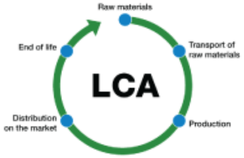
Target properties to generate key data

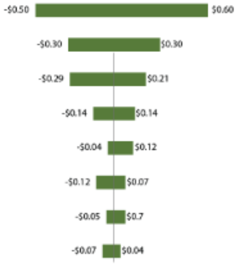
Conduct retrosynthetic analyses



Inform Analyses

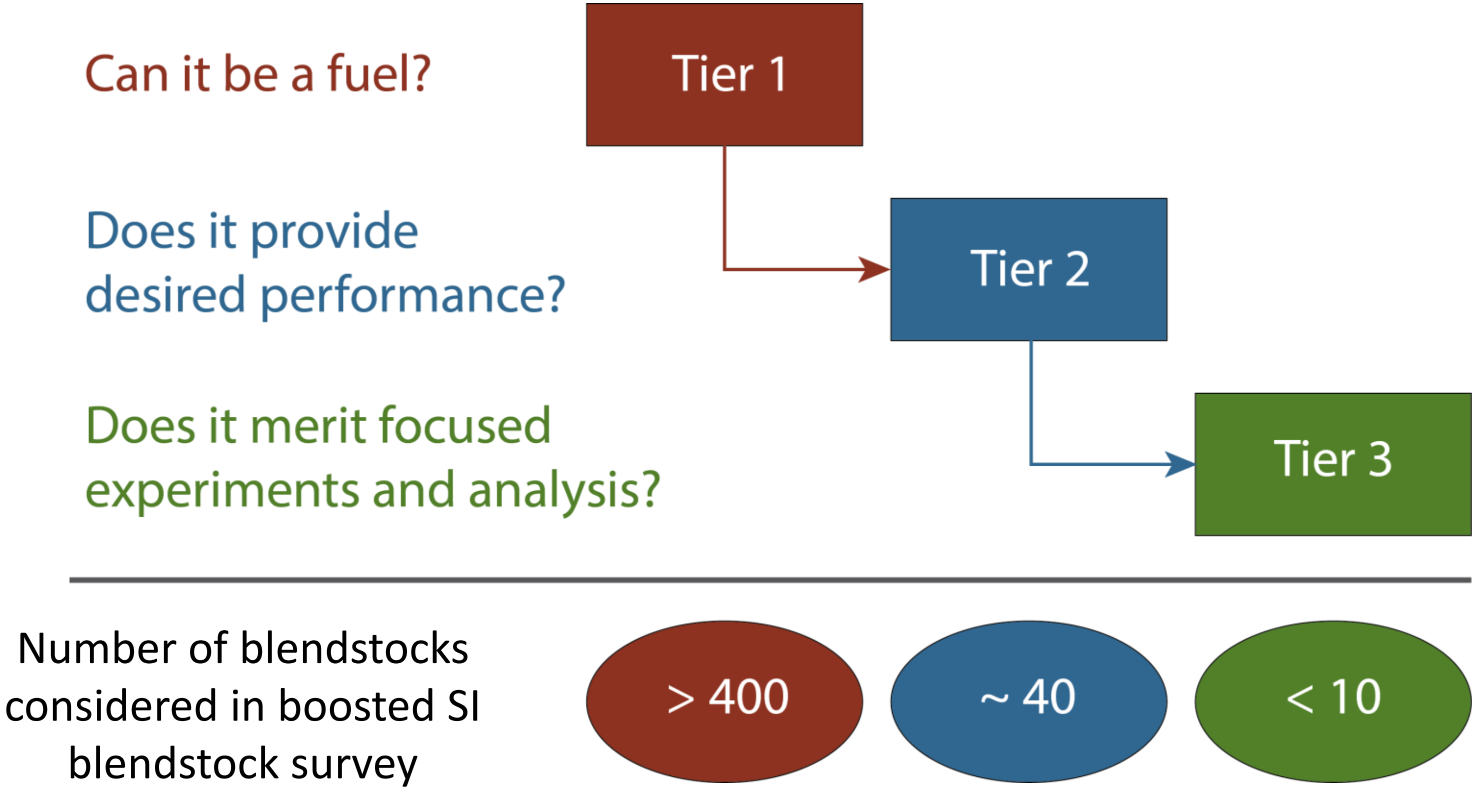
Provide improved data for LCA, TEA analyses





2 – Approach (Technical)

Tiered screening process is efficient, effective



Can it be a fuel?

Tier 1

Does it provide desired performance?

Tier 2

Does it merit focused experiments and analysis?

Tier 3

Number of blendstocks considered in boosted SI blendstock survey

> 400

~ 40

< 10

2 – Approach (Technical)

Analysis assesses benefits, barriers and impacts

Technology Readiness

State of technology: Fuel production

State of technology: Vehicle use

Conversion technology readiness level

Feedstock sensitivity

Process robustness

Feedstock quality

# of viable pathways

Environmental

Carbon efficiency

Target yield

Life cycle greenhouse gas emissions

Life cycle water

Life cycle fossil energy use

Economics

Target cost

Needed cost reduction

Co-product economics

Feedstock cost

Alternative high-value use

Other Factors

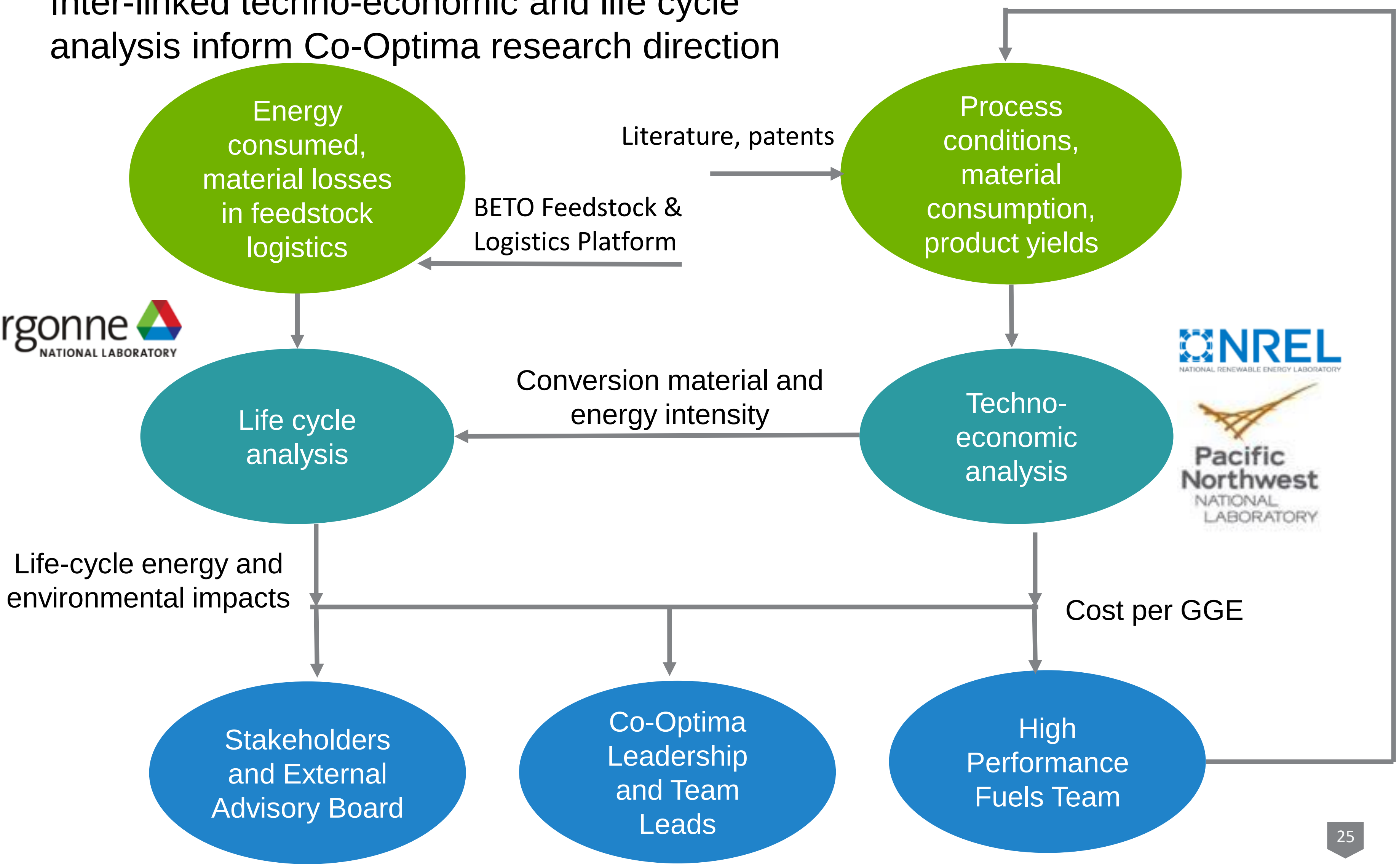
Geographic factors

Vehicle compatibility

Infrastructure compatibility

2 –Approach (Technical)
Analysis informs R&D across scales

Inter-linked techno-economic and life cycle analysis inform Co-Optima research direction



Energy consumed, material losses in feedstock logistics

Literature, patents

Process conditions, material consumption, product yields

BETO Feedstock & Logistics Platform

Life cycle analysis

Conversion material and energy intensity

Techno-economic analysis

Life-cycle energy and environmental impacts

Cost per GGE

Stakeholders and External Advisory Board

Co-Optima Leadership and Team Leads

High Performance Fuels Team

2 – Approach (Technical)

Key barriers and critical success factors identified

Critical success factors

- Must identify multiple blendstock options for successful engine-fuel combinations
- Blendstocks must demonstrate synergistic blending for high value to stakeholders
- Techno-economics and ***value*** must meet market needs
- Lifecycle emissions impacts must meet advanced biofuel criteria

Barriers

- Knowledge gaps complicate work staging
  - Structure-property relationships and blendstock discovery require fuel property knowledge
  - Blendstock evaluation precedes analysis tasks
- Balancing stakeholder input may require tradeoffs
- Early stage of R&D increases analysis uncertainty and makes estimating production costs challenging

2 – Approach (Technical)

Risks identified and mitigation plan in place

Risk Description	Response Plan	Severity	Probability	Classification
Fuel properties and target values critical to MM combustion not defined early in FY19 via VTO-funded Global Sensitivity Analysis	Shift resources to MCCI while analysis is completed	High	High	Schedule
Fuel properties and target values critical to KC combustion not defined early in FY20	Postpone initiation of KC fuel R&D	Moderate	Moderate	Schedule
Soot reduction sought for MCCI not realized in conventional engine	Terminate non-DFI* element of MCCI project	High	Low	Scope
Analysis indicates low expected uptake of new fuel and engine technologies	Refocus efforts on market barriers	Moderate	High	Scope

*DFI = ducted fuel injection

2- Approach (Management)

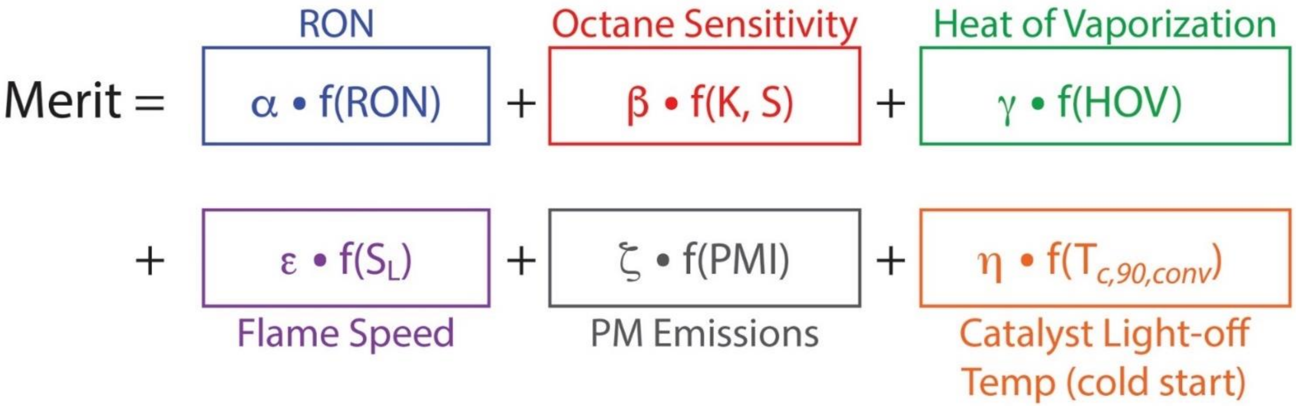
Milestones drive critical R&D

Selected FY19 milestones (of 34 total):

Task	Due	Title
A.4.5	Q4	Determine fuel properties for synthesized ether structures derived from reductive etherification of ketones and alcohols
A.4.10	Q4	Complete polymer exposure studies on selected MCCI blendstocks
A.5.1	Q4	Quantify impact of structural features of fuel candidates containing alcohol and ether functional groups for octane and phi sensitivity impacts
A.5.1	Q4	Identify the blendstock molecular structures or individual BOB component that leads to the highest antagonistic blending effect to raise RON and S
A.5.2	Q2	Develop production POC data along with fuel property verification for short-chain unsaturated alcohol(s)
A.5.6	Q3	Identify 5 new compounds or mixtures that improve octane sensitivity when blended into BOB or E10
B.3.13	Q4	Complete screening of 8-12 bio-blendstocks so that the Co-Optima team is informed of their scalability and economic and environmental viability
B.4.1	Q1	Report parameters, methodology, and results for feedback of bounding analysis to COLT for feedback prior to finalizing analysis
F.1.4.2	Q4	Develop prediction tool-kits from molecular structure for LDSI, MM blendstocks for physical and chemical properties important to dilution tolerance and flame speed

3 – Progress

Merit function used to compare Boosted SI blendstocks



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

RON = Research Octane Number; MON = Motor Octane Number; Sensitivity = RON – MON
HOV = Heat of Vaporization; S_L = Flame Speed; PMI = Particulate Matter Index

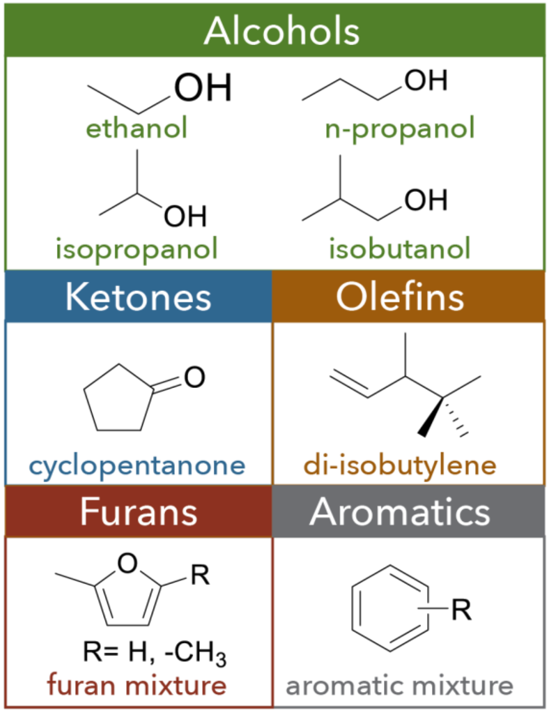
Reports released February 2018: https://energy.gov/eere/articles/co-optimization-engines-fuels-breakthrough-research-engine-and-fuel-co-optimization

Quantifies impact of fuel properties on engine efficiency developed and used to evaluate bio-blendstocks

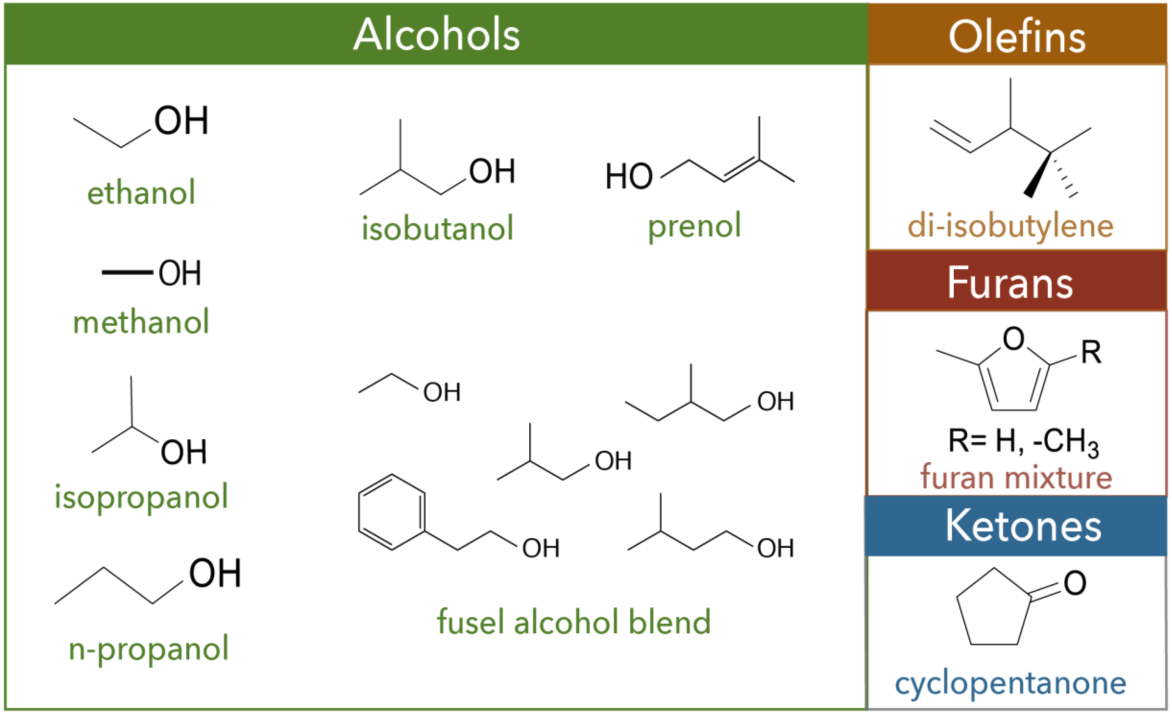
3 – Progress

Identified boosted SI blendstocks with highest potential

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



Blendstocks with highest merit function score

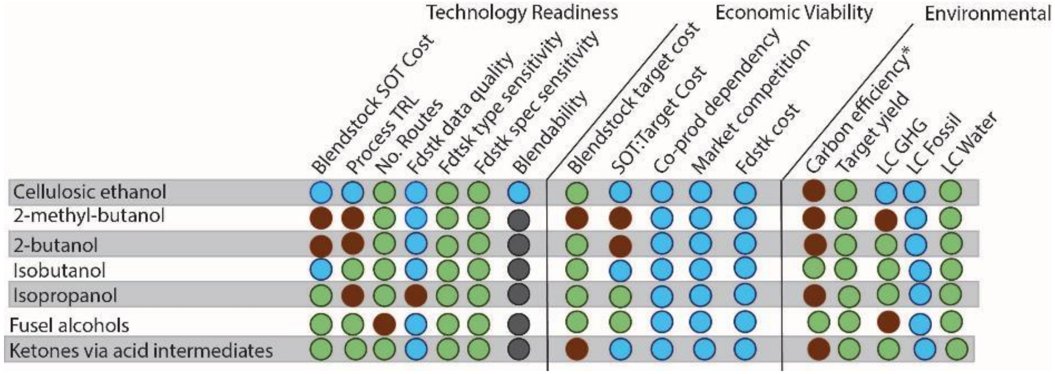


*Fusel alcohol blend: 57% isobutanol, 15% phenyl ethanol, 12% 3-methyl-1-butanol, 10% ethanol, 6% 2-methyl-1-butanol

Ten biomass-derived blendstocks show highest engine efficiency merit function score and predicted engine efficiency increase

3 – Progress

Completed economic, environmental, scalability analysis

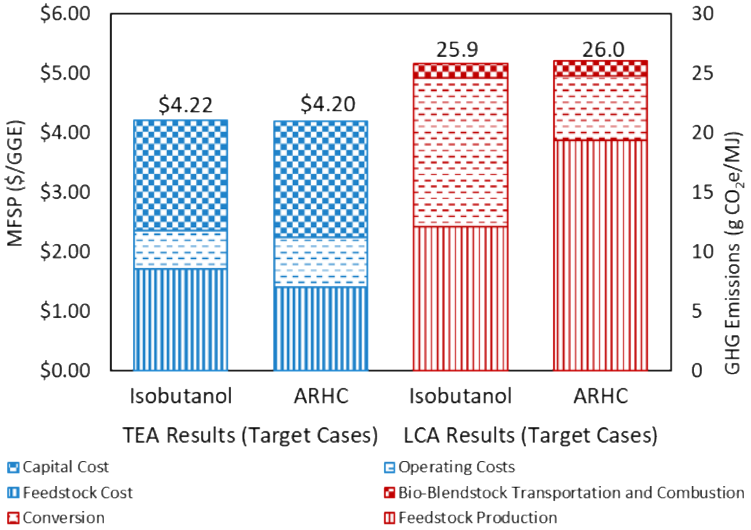


	Technology Readiness							Economic Viability					Environmental				
	Blendstock SOT Cost	Process TRL	No. Routes	Fdstk data quality	Fdtsk type sensitivity	Fdstk spec sensitivity	Blendability	Blendstock target cost	SOT:Target Cost	Co-prod dependency	Market competition	Fdstk cost	Carbon efficiency*	Target yield	LC GHG	LC Fossil	LC Water
Cellulosic ethanol	🔵	🔵	🟢	🔵	🟢	🟢	🔵	🟢	🔵	🔵	🔵	🔵	🟤	🟢	🔵	🔵	🟢
2-methyl-butanol	🟤	🟤	🟢	🔵	🟢	🟢	⚫	🟤	🟤	🔵	🔵	🔵	🟤	🟢	🟤	🔵	🟢
2-butanol	🟤	🟤	🟢	🔵	🟢	🟢	⚫	🟢	🟤	🔵	🔵	🔵	🟤	🟢	🟢	🔵	🟢
Isobutanol	🔵	🟢	🟢	🔵	🟢	🟢	⚫	🟢	🔵	🔵	🔵	🔵	🟢	🟢	🟢	🔵	🟢
Isopropanol	🟢	🟤	🟢	🟤	🟢	🟢	⚫	🟢	🟢	🔵	🔵	🔵	🟤	🟢	🟢	🔵	🟢
Fusel alcohols	🟢	🟢	🟤	🔵	🟢	🟢	⚫	🟢	🟢	🔵	🔵	🔵	🟢	🟢	🟤	🔵	🟢
Ketones via acid intermediates	🟢	🟢	🟢	🔵	🟢	🟢	⚫	🟤	🔵	🔵	🔵	🔵	🟤	🟢	🟢	🔵	🟢

Blue: Favorable, Green: Neutral, Brown: Unfavorable, Gray: Inconclusive

Screened
24 bio-blendstocks
for boosted SI

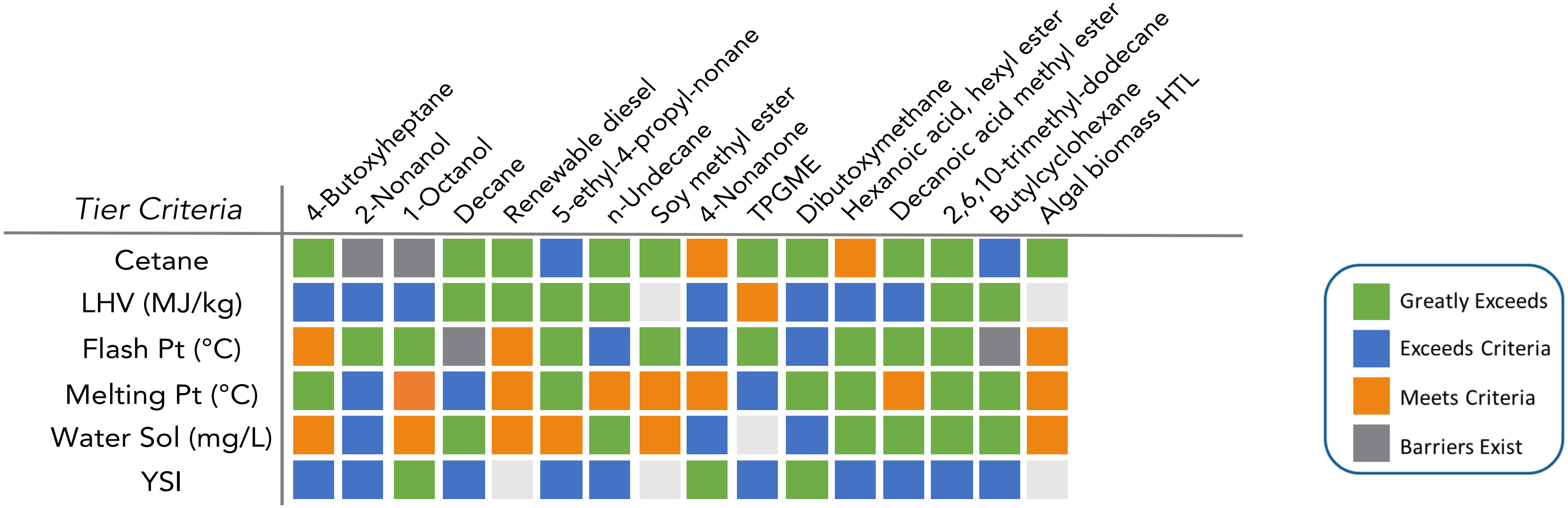
Detailed TEA and LCA of subset of bio-blendstocks



Evaluations help guide R&D at early stages and assess impacts at later stages

3 – Progress

Initial MCCI bio-blendstock screening complete



Tier Criteria	4-Butoxyheptane	2-Nonanol	1-Octanol	Decane	Renewable diesel	5-ethyl-4-propyl-nonane	n-Undecane	Soy methyl ester	4-Nonanone	TPGME	Dibutoxymethane	Hexanoic acid, hexyl ester	Decanoic acid methyl ester	2,6,10-trimethyl-dodecane	Butylcyclohexane	Algal biomass HTL
Cetane	🟩	⬛	⬛	🟩	🟩	🟦	🟩	🟩	🟧	🟩	🟩	🟧	🟩	🟩	🟦	🟩
LHV (MJ/kg)	🟦	🟦	🟦	🟩	🟩	🟩	🟩		🟦	🟧	🟦	🟦	🟦	🟩	🟩	
Flash Pt (°C)	🟧	🟩	🟩	⬛	🟧	🟩	🟦	🟩	🟦	🟩	🟦	🟩	🟩	🟩	⬛	🟧
Melting Pt (°C)	🟩	🟦	🟧	🟦	🟧	🟩	🟧	🟧	🟧	🟦	🟩	🟩	🟧	🟩	🟩	🟧
Water Sol (mg/L)	🟧	🟦	🟧	🟩	🟧	🟧	🟩	🟧	🟦		🟦	🟩	🟩	🟩	🟩	🟧
YSI	🟦	🟦	🟩	🟦		🟦	🟦		🟩	🟦	🟩	🟦	🟦	🟦	🟦	

🟩 Greatly Exceeds
🟦 Exceeds Criteria
🟧 Meets Criteria
⬛ Barriers Exist

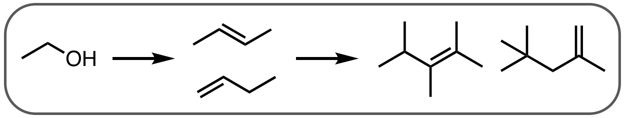
Numerous bio-derived oxygenates and paraffins reduce MCCI sooting potential and meet other targets; matching diesel energy density is a challenge

3 – Progress
Controlling autoignition key to MM combustion

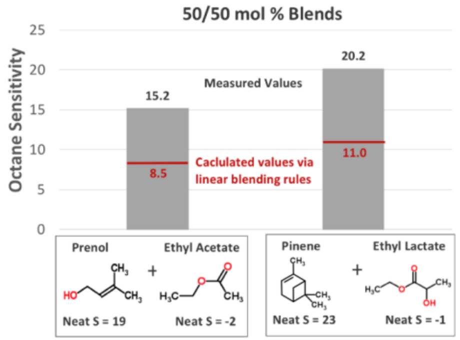
Initial set of critical MM fuel properties

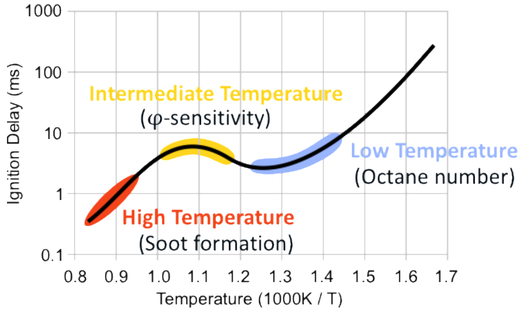
BP	Boiling point	~Gasoline range T_{10}, T_{50}, T_{90}
RON	Research octane number	Boosted SI operation under high load
S	Octane sensitivity	Reactivity at high T
Φ_S	Phi sensitivity	Tune ignition via charge stratification
S_L	Laminar flame speed	Higher S_L increases dilution tolerance

Example Ethanol to Iso-Olefin Pathway



Producing iso-olefins for Φ_S testing





Developing structure-property relationships

Developing S and Φ_S structure-property relationships and identifying candidate bio-blendstocks providing high S, Φ_S to tune autoignition control

3 – Technical Accomplishments

Key findings are documented for stakeholders

- Published >110 papers, 1 patent, >90 presentations
- DOE reports
- Annual year-in-review summary documents

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

Co-Optimization of Fuels & Engines

Misfueling Mitigation

FY18 YEAR IN REVIEW

CO-OPTIMIZATION OF FUELS & ENGINES

U.S. DEPARTMENT OF ENERGY | Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

FY16 Year in Review

better fuels | better vehicles | sooner

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

FY16 YIR: https://www.nrel.gov/docs/fy17osti/67595.pdf
FY17 YIR: https://www.energy.gov/sites/prod/files/2018/04/f50/Co-Optima_YIR2017_FINAL_Web_180417_0.pdf
FY18 YIR to be published

3 – Progress

Major FY16-18 results captured in Year in Review (1 of 2)

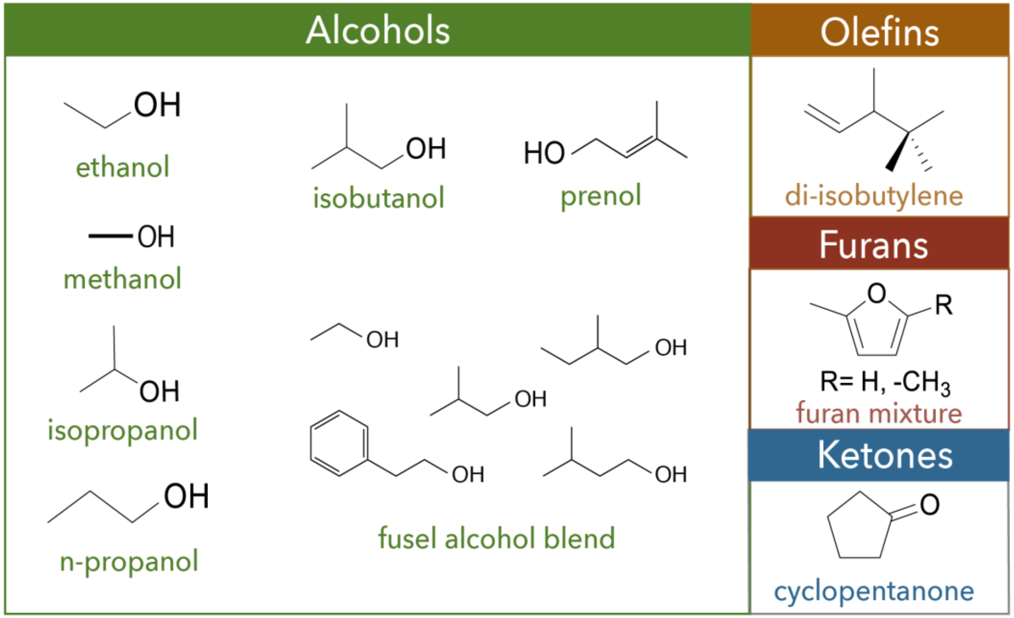
Fuel

- Identified 10 blendstocks with highest merit function scores
- Identified 6 blendstocks with highest merit function scores and fewest barriers to market
- Identified chemical families which may provide fuel properties needed for high efficiency SI and lower emission MCCI engines
- Formulated structure-activity relationships that describe how chemical functional groups impart important properties to fuels
- Identified blendstocks for SI engines with beneficial, non-linear blending behavior
- Evaluated barriers to adoption, including infrastructure, engine and production pathway elements

Tools

- Developed new models, numerical algorithms and computational tools that accelerate R&D

Blendstocks with highest merit function score



3 – Progress

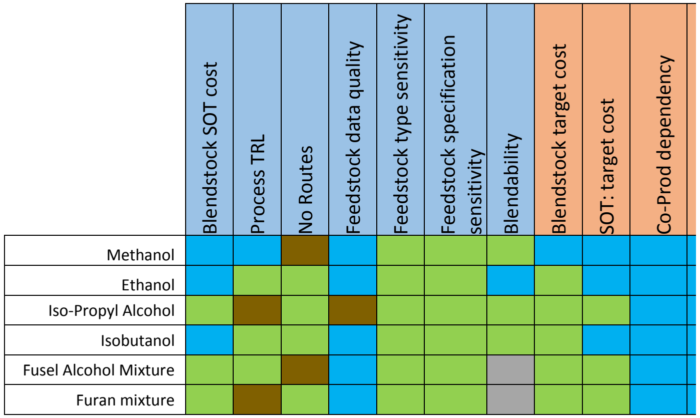
Major FY16-18 results captured in Year in Review (2 of 2)

Analysis

- Identified blendstocks with near-term commercial potential through comparative systems-level analyses of 23 metrics representing economic, environmental, technology, and market factors
- Conducted benefits analysis to estimate key performance indicators such as carbon emissions reductions, jobs, and
- Evaluated refinery integration opportunities to identify opportunities to capture enhanced bioblendstock value
- Estimated savings from MCCI soot emissions reduction

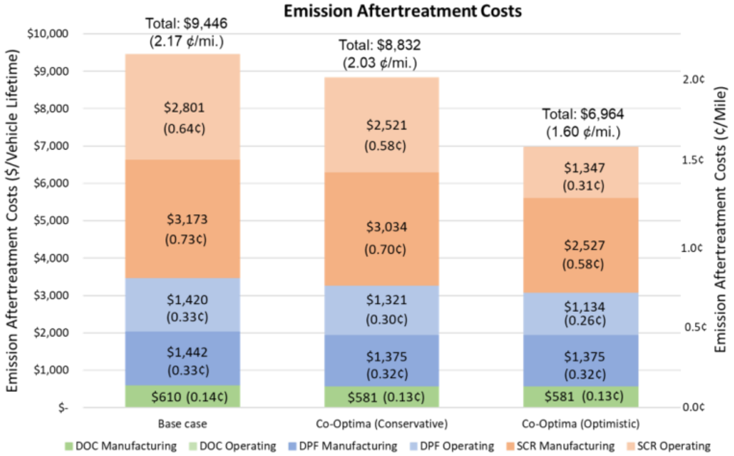
Combustion

- Provided new understanding of how fuel chemistry can enable highly efficient boosted SI operation
- Developed Merit Function for turbocharged gasoline engines – much more accurate predictor of engine efficiency than previous methods
- Advanced low soot MCCI fuel injection technology



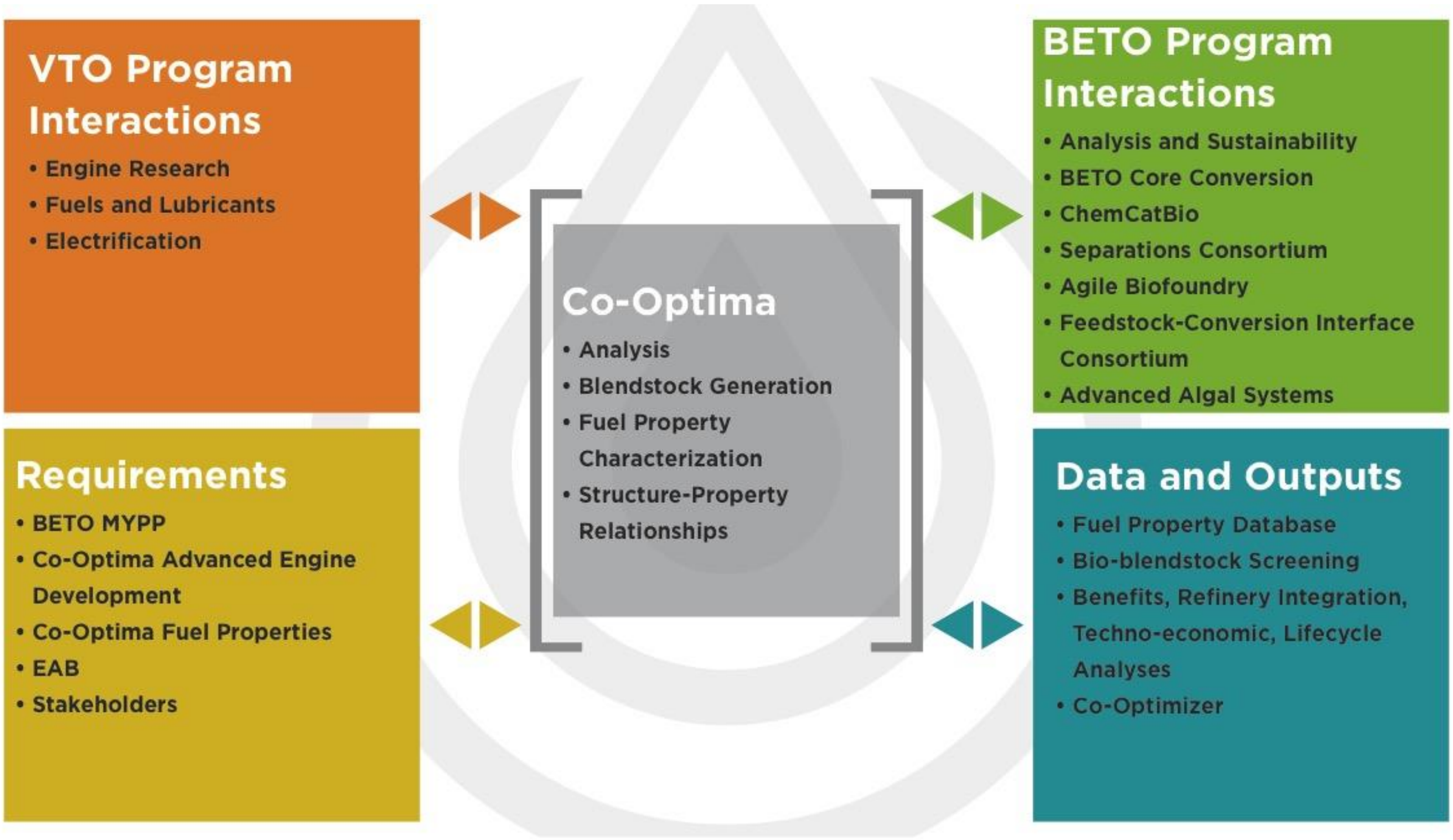
	Blendstock SOT cost	Process TRL	No Routes	Feedstock data quality	Feedstock type sensitivity	Feedstock specification sensitivity	Blendability	Blendstock target cost	SOT: target cost	Co-Prod dependency
Methanol	🟦	🟦	🟫	🟦	🟩	🟩	🟩	🟦	🟦	🟦
Ethanol	🟦	🟩	🟩	🟦	🟩	🟩	🟦	🟩	🟦	🟦
Iso-Propyl Alcohol	🟩	🟫	🟩	🟫	🟩	🟩	🟩	🟩	🟩	🟦
Isobutanol	🟦	🟩	🟩	🟦	🟩	🟩	🟩	🟩	🟦	🟦
Fusel Alcohol Mixture	🟩	🟩	🟫	🟦	🟩	🟩	⬜	🟩	🟩	🟦
Furan mixture	🟩	🟫	🟩	🟦	🟩	🟩	⬜	🟩	🟩	🟦

Note 1: Blue, green, and Brown boxes represent favorable, neutral, and unfavorable categorization



4 – Relevance

Connected to BETO and stakeholders



VTO Program Interactions

- Engine Research
- Fuels and Lubricants
- Electrification

Requirements

- BETO MYPP
- Co-Optima Advanced Engine Development
- Co-Optima Fuel Properties
- EAB
- Stakeholders

Co-Optima

- Analysis
- Blendstock Generation
- Fuel Property Characterization
- Structure-Property Relationships

BETO Program Interactions

- Analysis and Sustainability
- BETO Core Conversion
- ChemCatBio
- Separations Consortium
- Agile Biofoundry
- Feedstock-Conversion Interface Consortium
- Advanced Algal Systems

Data and Outputs

- Fuel Property Database
- Bio-blendstock Screening
- Benefits, Refinery Integration, Techno-economic, Lifecycle Analyses
- Co-Optimizer

4 – Relevance
Co-Optima is integral BETO strategy component

ADO-E. Co-Development of Fuels and Engines: "…advanced engine development efforts are constrained by the fuels in the market today. [Co-optimization]….potential to increase vehicle engine efficiency, improve fuel economy, and reduce emissions…requires improved understanding of…fuel properties…and what…properties can be provided by biofuel blendstocks.

Co-Optima is identifying **what** fuel properties enable highly efficient and clean engines.

- Identifies critical fuel properties (Merit Function)
- Identifies specific targets (structure-fuel property relationships)
- Provides retro-synthetic analysis that connect to BETO and other pathways

Complements BETO's focus on what "processing components" could be used to produce bio-blendstocks

Addresses what does an engine want and what should we make

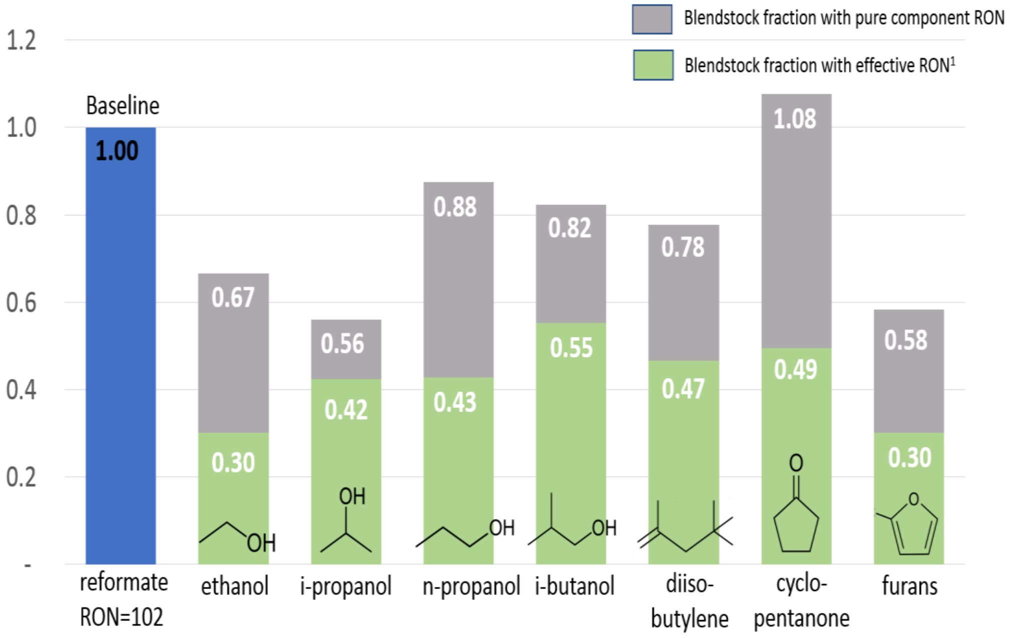
Impact: Plays a critical role in BETO strategy, provides options for producers in a way that does not pick winners

4 – Relevance
Results inform stakeholders

At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts: Biofuels and bioproducts…offer performance advantages relative to other technology options…Ongoing, forward-looking analyses…to identify these opportunities…R&D priorities can be adjusted appropriately.

Co-Optima’s fundamentally different approach identifies new opportunities for biomass-derived blendstocks offering

- Improved properties new value throughout supply chain
- Assessment of impacts
- Guidance to market actors across supply chain



Impact: Performance-driven improved value proposition

4 – Relevance
Enables higher efficiency and performance

From strategic plan "Co-optimization of fuels and engines offers the potential to significantly improve vehicle engine efficiency, maximize engine performance and carbon efficiency, … through accelerating the widespread deployment of improved fuels and engines."

Co-Optima is developing science that provides new value propositions and supports market pull

- Assessing how fuel properties extend the range of efficiency across the speed-load drive cycle
- Targeting bio-blendstocks that offer improvements over petroleum-derived fuels

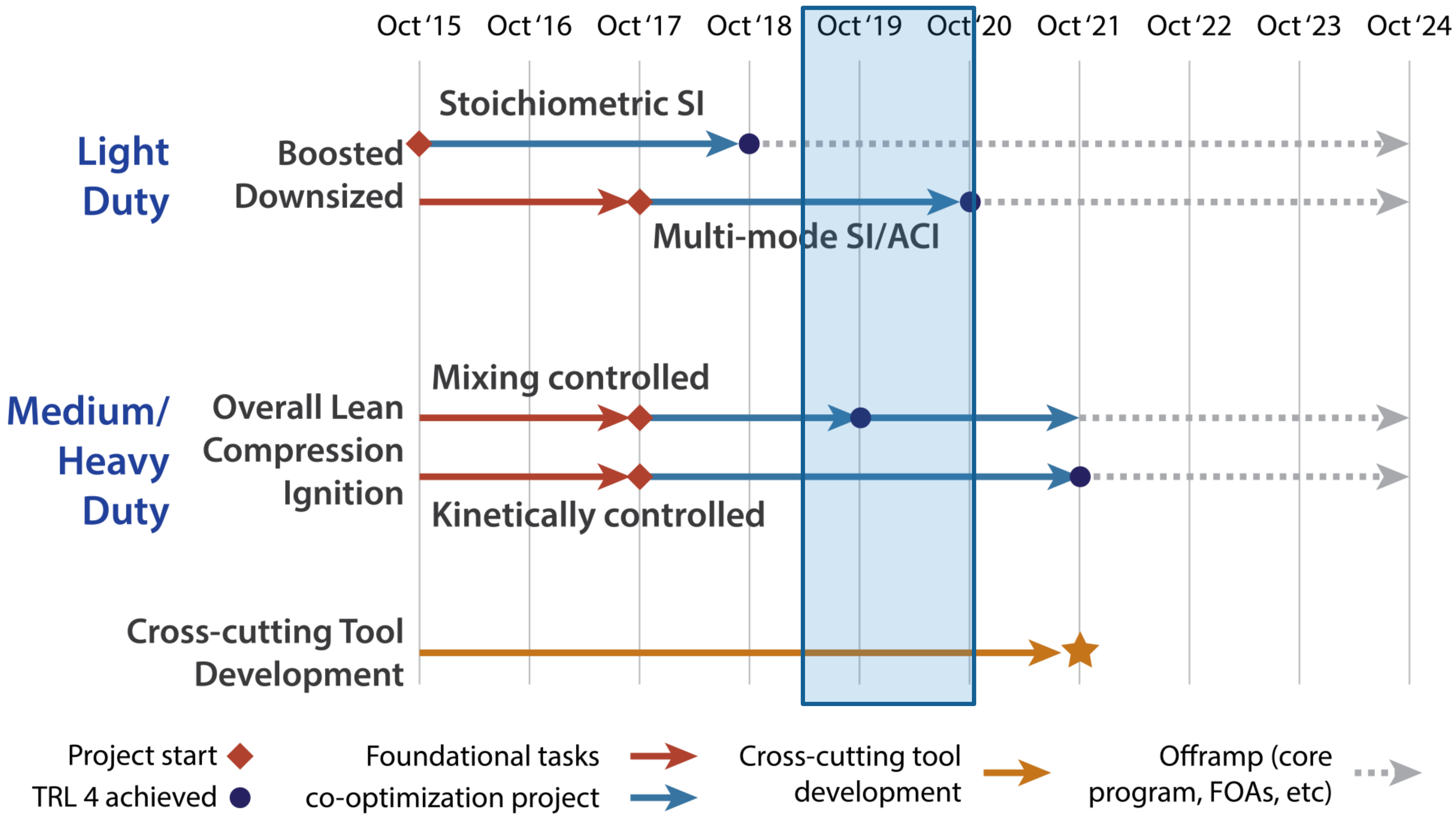
Co-Optima is addressing fuel deployment

- Determining the blending behavior of the bio-blendstocks within a petroleum matrix
- Understanding impact on infrastructure (engines, fuel transport and storage)
- Producing property-based fuel specifications

Impact:
market pull

5 – Future Work

Look ahead at next 18 months



5 – Future Work (MCCI)

Identify, quantify critical fuel property requirements

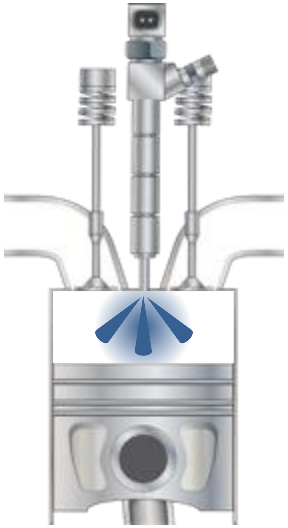
Outcomes

- Heavy-duty vehicle and fuels value proposition
- Merit table defining key fuel properties and target values
- Determine oxygenated fuel impacts on ducted fuel injection (DFI) emissions
- Final list of blendstocks possessing target values of critical fuel properties
- TEA, LCA, and refinery benefits analyses establishing potential value
- Confirmation of NO_x and PM reduction potential

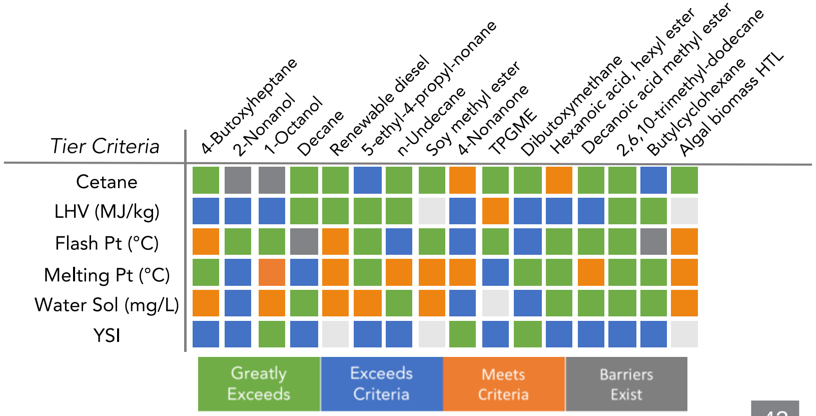
MYP Milestone Addressed:

By 2019, identify…10 promising bio-based blendstocks…[which]…decrease criteria pollutant emissions [and improve] key fuel properties (such as cold flow properties, energy density, and cetane number).

Nearly complete by FY19 end



Mixing-Controlled Compression Ignition



Tier Criteria	4-Butoxyheptane	2-Nonanol	1-Octanol	Decane	Renewable diesel	5-ethyl-4-propyl-nonane	n-Undecane	Soy methyl ester	4-Nonanone	TPGME	Dibutoxymethane	Hexanoic acid, hexyl ester	Decanoic acid methyl ester	2,6,10-trimethyl-dodecane	Butylcyclohexane	Algal biomass HTL
Cetane	🟩	⬛	⬛	🟩	🟩	🟦	🟩	🟩	🟧	🟩	🟩	🟧	🟩	🟩	🟦	🟩
LHV (MJ/kg)	🟦	🟦	🟦	🟩	🟩	🟩	🟩	⬜	🟦	🟧	🟦	🟦	🟦	🟩	🟩	⬜
Flash Pt (°C)	🟧	🟩	🟩	⬛	🟧	🟩	🟦	🟩	🟦	🟩	🟦	🟩	🟩	🟩	⬛	🟧
Melting Pt (°C)	🟩	🟦	🟧	🟦	🟧	🟩	🟧	🟧	🟧	🟦	🟩	🟩	🟧	🟩	🟩	🟧
Water Sol (mg/L)	🟧	🟦	🟧	🟩	🟧	🟧	🟩	🟧	🟦	⬜	🟦	🟩	🟩	🟩	🟩	🟧
YSI	🟦	🟦	🟩	🟦	⬜	🟦	🟦	⬜	🟩	🟦	🟩	🟦	🟦	🟦	🟦	⬜

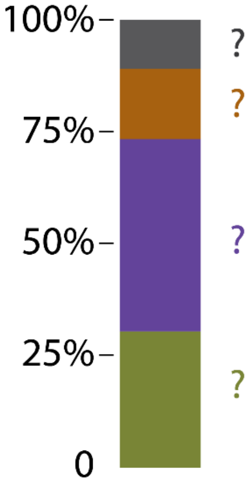
🟩 Greatly Exceeds
🟦 Exceeds Criteria
🟧 Meets Criteria
⬛ Barriers Exist

5 – Future Work (MM)

Identify, quantify critical fuel property requirements

Decision Point end of FY20

Multi-mode SI/ACI



Current research is identifying relative importance of key fuel properties

Outcomes

- Determine a means for assessing fuel property merit and determine target fuel property values and ranges
- Quantify relationships between fuel properties and engine parameters for combustion approaches
- Develop list of blendstocks possessing fuel properties in target range
- Conduct TEA, LCA, and refinery benefits analysis to establish potential value
- Assess fuel economy improvement

MYP Milestone: By 2030, demonstrate a simulated 35% improvement in passenger vehicle fuel economy (relative to a 2015 baseline) resulting from co-optimized fuels and engines utilizing bioblendstocks with tailored properties.

5 – Future Work (Kinetically-Controlled CI)

Identify, quantify critical fuel property requirements

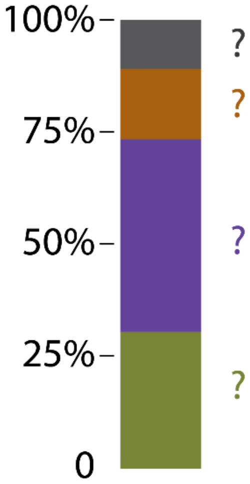
Outcomes

- Identify full-map combustion approaches and fuel-centered design criteria
- Assessment of fuel property impacts on KC engine operational constraints
- Develop an approach to assess merit of fuel properties
- Determine target values of fuel properties and ranges for each combustion approach

MYP Milestone: By 2023, identify at least 10 promising bio-based blendstocks…for use in a kinetically controlled compression ignition engine with the potential to decrease criteria pollutant emission and boost fuel economy by up to 4% in heavy-duty vehicles.

Decision Point by FY21 end

Kinetically Controlled



Current research is identifying approach to determine fuel properties and assess merit

5 – Future Work

Go/No Go Milestone (3/31/2020)

Multimode Milestones

1. Identify quantitative relationship between fuel properties (e.g., RON, S, HoV, S_L, volatility) and engine parameters (e.g., thermal stratification, injection strategy) with compression ignition combustion phasing (CA50) and shape of heat release curve [VTO]

2. Identify at least three bio-blendstocks that exhibit target values of these properties and meet advanced biofuel criteria, including at least 60% reduction in lifecycle carbon emissions and volumetric cost-performance parity with petroleum reformate [BETO]

Criteria

1. Mathematical relationship between RON, S, HoV, S_L, volatility and engine parameters
2. Three bioblendstocks meeting all 5 critical fuel property requirements and 60% carbon emissions reduction

Summary

Overview	**Develop new fuel and combustion options for more efficient engines with lower harmful emissions, resulting in market pull for the transport sector.**
Approach	• Multi-discipline, multi-office effort • Hypothesis-driven fuel property-based approach • Constrain combustion options and co-optimize renewable fuel blendstocks • Light and heavy duty on-road fleets • Output informs industry stakeholders
Technical Progress	• Developed engine efficiency merit function • Assembled publicly accessible fuel property database • Identified 10 most promising boosted SI candidates • Measured blending behavior of chemically diverse bio-blendstocks • Completed initial life-cycle analysis of >20 bio-blendstock options • Completed light-duty benefits, refinery integration analyses
Relevance	• Provides technical basis for evaluating bio-blendstocks • Identifies key bio-blendstocks that enable engines to operate cleanly and efficiently • Identifies what fuels engines want and compliments BETO pathway approach • Developing performance and pathway to enable technical analyses
Future Work	• Complete MCCI (diesel) blendstock evaluation • Identify MM bio-blendstocks enabling efficient operation • Determine KC blendstock options • Evaluate benefits and impacts of MCCI, MM and KC fuel-engine combinations

Acronyms (1 of 2)

ACI – Advanced compression ignition

AED – Advanced Engine Development team

ANL – Argonne National Laboratory

ASSERT – Analysis of Sustainability, Scale, Economics, Risk and Trade team

BETO – Bioenergy Technologies Office

CA50 – crank angle position where 50% of the heat is released

CI – Compression ignition

COLT – Co-Optima leadership team

DFI – ducted fuel injection

DOE – Department of Energy

EAB – external advisory board

EERE – DOE Office of Energy Efficiency and Renewable Energy

EPA – Environmental Protection Agency

FE – fuel economy

FP – Fuel Properties team

GGE – gallon of gas equivalent

GHG – greenhouse gas

HD – heavy

HoV – heat of vaporization

HPF – High Performance Tuel team

INL – Idaho National Laboratory

K – Kalghati K number

KC – kinetically-controlled combustion

LANL – Los Alamos National Laboratory

LBNL – Lawrence Berkeley National Laboratory

LC - lifecycle

LCA – lifecycle analysis

LD – Light duty

LFS – laminar flame speed

LHV – lower heating value

LLNL – Lawrence Livermore National Laboratory

MCCI – mixing-controlled compression ignition (e.g., diesel)

MM – multimode combustion

MON – motor octane number

NOx – nitrogen oxides

NREL – National Renewable Energy Laboratory

Acronyms (2 of 2)

OEM – original equipment manufacturer

ORNL – Oak Ridge National Laboratory

PM – particulate matter

PMI – particulate matter index

PNNL – Pacific Northwest National Laboratory

R&D – research and development

RON – research octane number

S – octane sensitivity (RON – MON)

SI – spark ignition

S_L – laminar flame speed

SNL – Sandia National Laboratories

SOT – state of technology

$T_{c,90,conv}$ – temperature at which 90% of criteria pollutants are converted to less harmful gases

TEA – techno-economic analysis

TK – Simulation Toolkit team

TRL – technology readiness level

USCAR – The United States Council for Automotive Research

VTO - Vehicle Technologies Office

WSU – Washington State University

WTW – well-to-wheels

XLT – extended leadership team

YIR – year in review

YSI – yield sooting index

Additional Slides

Responses to Previous Reviewers' Comments (1 of 2)

Reviewer comments:

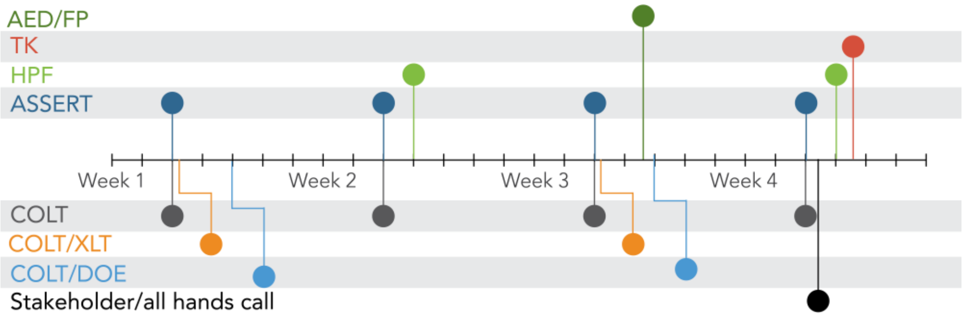
- No guarantee that industry will use information to provide better fuels.
- No plan of attack for impetus for industry change.
- Lots of calls and meetings

Response

- These risks are real. To mitigate these risks, Co-Optima has focused on extensive outreach to communicate the technical foundation we have developed, so that market actors can act. Our outreach plan includes direct engagement with biofuel companies at all scales, as well as with automakers and all parts of the fuel supply chain, including Octane Workshops in 2018 (next slide), and a concerted effort to solicit feedback from biofuels companies in 2018 (report is being drafted).
- We have made an effort to manage the work more efficiently, reducing the number of meetings across Co-Optima by 1/3, and reduced travel for the leadership team by another 1/3.

Co-Optima has improved efficiency and reduced meeting burden

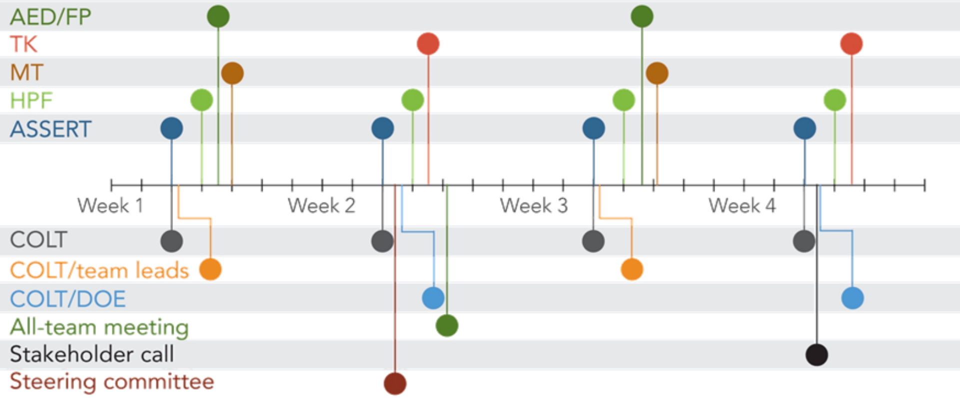
Co-Optima regularly scheduled meetings



Regular team meetings have cross-team participation

AED/FP: Advanced Engine Development/Fuel Properties; TK: Modeling and Simulation Toolkit; HPF: High Performance Fuels; ASSERT: Analysis of Sustainability, Scale, Economics, Risk, and Trade; COLT: Co-Optima Leadership Team; XLT: Extended Leadership Team (COLT, DOE, Steering Committe)

Co-Optima regularly scheduled meetings



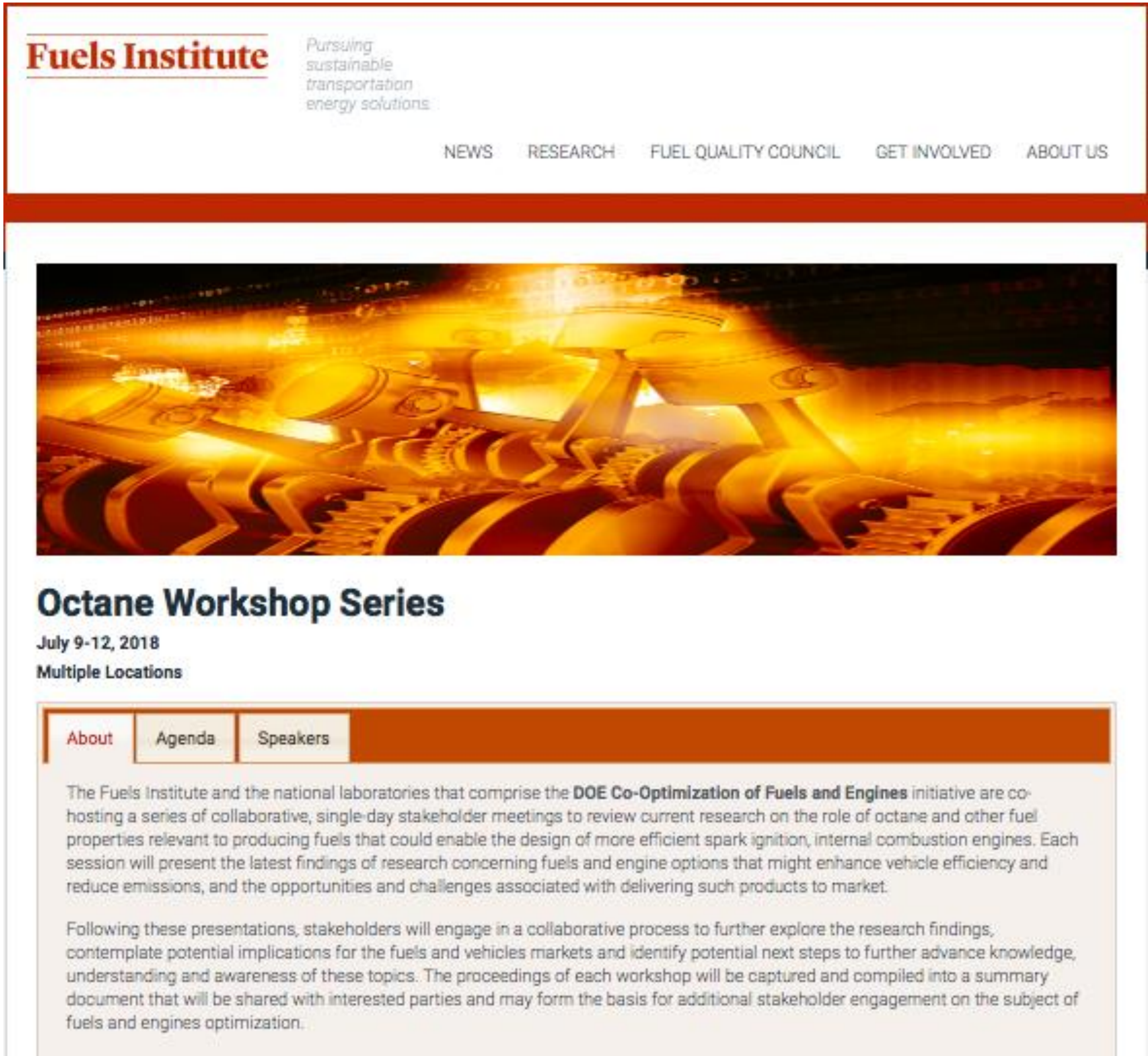
Weekly/biweekly team meetings have cross-team participation

AED/FP: Advanced Engine Development/Fuel Properties; TK: Modeling and Simulation Toolkit MT: Market Transformation; HPF: High Performance Fuels; ASSERT: Analysis of Sustainability, Scale, Economics, Risk, and Trade; COLT: Co-Optima Leadership Team

From 25 to 17 meetings per month

Responses to Previous Reviewers' Comments (2 of 2)

Conducted with Fuels Institute at two sites



Octane Workshop Series

July 9-12, 2018

Multiple Locations

The Fuels Institute and the national laboratories that comprise the **DOE Co-Optimization of Fuels and Engines** initiative are co-hosting a series of collaborative, single-day stakeholder meetings to review current research on the role of octane and other fuel properties relevant to producing fuels that could enable the design of more efficient spark ignition, internal combustion engines. Each session will present the latest findings of research concerning fuels and engine options that might enhance vehicle efficiency and reduce emissions, and the opportunities and challenges associated with delivering such products to market.

Following these presentations, stakeholders will engage in a collaborative process to further explore the research findings, contemplate potential implications for the fuels and vehicles markets and identify potential next steps to further advance knowledge, understanding and awareness of these topics. The proceedings of each workshop will be captured and compiled into a summary document that will be shared with interested parties and may form the basis for additional stakeholder engagement on the subject of fuels and engines optimization.

Lessons Learned from Go/No Go

- Two governing hypotheses were confirmed (within limits of applicability determined within Co-Optima – engine conditions between RON and MON, inclusive)
- RON and S provide 85-95% of engine efficiency increase under turbocharged conditions
  - S less important under naturally-aspirated conditions
- Synergistic blending performance key to bio-blendstock value
- Some level of infrastructure compatibility essential to techno-economics and value proposition to stakeholders

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

Publications & Presentations (1)

125+ publications, 100+ presentations, 1 patent

FY19:

- **Oligomerization of Ethanol-Derived Propene and Isobutene Mixtures to Transportation Fuels: Catalyst and Process Considerations** – J. Saavedra, R. A Dagle, V. Dagle, C. Smith, K. O. Albrecht, *Catal. Sci. & Tech.,* 2019, DOI: 10.1039/C8CY02297F.
- **Discovery of novel octane hyperboosting phenomenon in prenol/gasoline blends –** E. Monroe; J. Gladden; K. O. Albrecht; J. T. Bays; R. L. McCormick; R. W Davis; A. George. *Fuel*, V.239, 1143-1148, 2019.
- **Heat of Vaporization and Species Evolution During Gasoline Evaporation Measured by DSC/TGA/MS for Blends of C1 to C4 Alcohols in Commercial Gasoline Blendstocks –** G. Fiorini, E. Christensen, L. Fouts, R. L. McCormick, SAE Technical Paper 2019-01-0014, 2019. doi:10.4271/2019-01-0014
- **Measurement of Heat of Vaporization for Research Gasolines and Ethanol Blends by DSC/TGA –** G. Fiorini, L. Fouts, E. Christensen, J. E. Anderson, R. L. McCormick, Energy Fuels, 32(12), 12607-12616, 2018. DOI: 10.1021/acs.energyfuels.8b03369.
- **Estimation of the Fuel Efficiency Potential of Six Gasoline Blendstocks Identified by the U.S. Department of Energy's Co-Optimization of Fuels and Engines Program** – S. Sluder, SAE Technical Paper 2019-01-0017, 2019.
- **Multi-fuel surrogate chemical kinetic mechanisms for real world applications -** C. K. Westbrook, M. Mehl, W. J. Pitz, G. Kukkadapu, S. Wagnon and K. Zhang, Phys. Chem. Chem. Phys. 20 (16) (2018) 10588-10606. https://doi.org/10.1039/C7CP07901J
- **An experimental and kinetic modeling study of the oxidation of hexane isomers: Developing consistent reaction rate rules for alkanes** – K. Zhang, C. Banyon, U. Burke, G. Kukkadapu, S. W. Wagnon, M. Mehl, H. J. Curran, C. K. Westbrook and W. J. Pitz, *Combust. Flame,* In press, (2019).
- **Multi-functional Mixed Oxide Catalysis in Cascade Chemistry to Convert Ethanol to C5+ Ketones –** S. Subramaniam, K. Lin, M. Guo, and K. Kallupalayam Ramasamy. Presented at AIChE Annual Meeting, Pittsburgh, Pennsylvania, 11/2018.

Publications & Presentations (2)

- **Short-chain ketone production by engineered polyketide synthases in Streptomyces albus –** S. Yuzawa, M. Mirsiaghi, R. Jocic, T. Fujii, F. Masson, V. T. Benites, E. E. K. Baidoo, E. Sundstrom, D. Tanjore, T. R. Pray, A. George, R. W. Davis, J. M. Gladden, B. A. Simmons, L. Katz and J. D. Keasling, *Nature Communications* 9, Article number: 4569 (2018). https://doi.org/10.1038/s41467-018-07040-0
- **Measuring and Predicting the Vapor Pressure of Gasoline Containing Oxygenates** – D. J. Gaspar; S. D. Phillips; E. Polikarpov;, K. O. Albrecht; S. B. Jones; A. George; A. Landera; D. M. Santosa; D. T. Howe; A. G. Baldwin; J. T. Bays, *Fuel*, 2019, accepted.
- **Insights into engine autoignition: Combining engine thermodynamic trajectory and fuel ignition delay iso-contour** – M. Tao, P. Zhao, J. Szybist, P. Lynch, H. Ge, *Combust. Flame*, 200 (2), 207-218, 2019. https://doi.org/10.1016/j.combustflame.2018.11.025
- **Critical Fuel Property Evaluation for Potential Gasoline and Diesel Biofuel Blendstocks with Low Sample Volume Availability –** E. Polikarpov, K. O. Albrecht, J. P. Page, D. Malhotra, P. Koech, L. Cosimbescu, D. J Gaspar. *Fuel* 238, 26-33, 2019. https://doi.org/10.1016/j.fuel.2018.09.129
- **A simple, solvent free method for transforming bio-derived aldehydes into cyclic acetals for renewable diesel fuels** – O. Staples, C. M. Moore, T. A Semelsberger, J. H. Leal, C. S. McEnally, L. Pfefferle, and A. D. Sutton, *Sustainable Energy Fuels*, 2018, Accepted Online https://doi.org/10.1039/C8SE00371H
- **Autoignition and select properties of low sample volume thermochemical mixtures from renewable sources** – M. V. Olarte, K. O. Albrecht, J. T. Bays, E. Polikarpov, B. Maddi, J. C. Linehan, M. J. O'Hagan, D. J. Gaspar, *Fuel* 238 493-506, 2019. https://doi.org/10.1016/j.fuel.2018.10.115
- **The impact of physicochemical property interactions of iso-octane/ethanol blends on ignition timescales –** C. L. Barraza-Botet, J. Luecke; B. T. Zigler; M. S. Wooldridge, *Fuel*, 224, 401-411, 2018. https://doi.org/10.1016/j.fuel.2018.03.105

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- **Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Mixing Controlled Compression Ignition Combustion – G**. M. Fioroni, L. Fouts, J. Luecke, D. Vardon, N. Huq, E. D. Christensen, X. Huo, T. L. Alleman, R. L. McCormick, M. Kass, E. Polikarpov, SAE Technical Paper 2019-01-0570 (2019).
- **Catalytic upgrading of short chain acids to renewable diesel fuel –** X. Huo, N.A. Huq, J. Stunkel, et al. Presented by D.R. Vardon at Frontiers in Biorefining, St. Simons Island, GA, 2019.
- **Catalytic Carbon Chain Extension and Selective Defunctionalization of Bioderived Building Blocks** – A. D. Sutton, presented at Frontiers in Biorefining, St Simmons Island, GA, 11/2018.
- **A Photochemical Approach to Generate Energy Dense Fuels from Biomass** – C. L. Ford, presented at Frontiers in Biorefining, St Simmons Island, GA, 11/2018.
- **Hydrodeoxygenation of Bio-derived Ketones With Heterogeneous Catalysts for Fuel and Chemical Production** – X. Yang, presented at Frontiers in Biorefining, St Simmons Island, GA, 11/2018.

Publications & Presentations (4)

FY18:

- **A Comprehensive Detailed Kinetic Mechanism for the Simulation of Transportation Fuels, 10th US National Combustion Meeting –** M. Mehl, S.W. Wagnon, K. Zhang, G. Kukkadapu, W.J. Pitz, C.K. Westbrook, Y. Zhang, H.J. Curran, N. Atef, M.J. Al Rashidi, M.S. Sarathy, and A. Ahmed. Paper 1A17, 2017. https://www.osti.gov/biblio/1357381-comprehensive-detailed-kinetic-mechanism-simulation-transportation-fuels
- **A Machine Learning-Genetic Algorithm (ML-GA) Approach for Rapid Optimization Using High-Performance Computing –** A.A. Moiz, P. Pal, D. Probst, Y. Pei, Y. Zhang, S. Som, J. Kodavasal. SAE Technical Paper 2018-01-0190, 2018. https://doi.org/10.4271/2018-01-0190
- **A New Chemical Kinetic Method of Determining RON and MON Values for Single Component and Multicomponent Mixtures of Engine Fuels –** C.K. Westbrook, M. Sjöberg, and N.P. Cernansky. Combustion and Flame, 195:50-62, April 2018. https://doi.org/10.1016/j.combustflame.2018.03.038
- **A Recent Progress of Rapid Compression Machine Works: Quantifying Fuel Reactivity for Model Validation and Fuel Ranking –** D. Kang and S. Goldsborough. Presented to the AEC MOU, Southfield, Michigan, August 15, 2018.
- **A Simple, Solvent Free Method for Transforming Bio-Derived Aldehydes into Cyclic Acetals for Renewable Diesel Fuels –** O. Staples, C.M. Moore, T.A. Semelsberger, J.H. Leal, C.S. McEnally, L. Pfefferle and A.D. Sutton. Sustainable Energy Fuels, 2018. https://doi.org/10.1039/C8SE00371H
- **An Experimental, Theoretical, and Modeling Study of the Ignition Behavior of Cyclopentanone –** B.K. Zhang, N. Lokachari, E. Ninnemann, S. Khanniche, W.H. Green, H.J. Curran, S.S. Vasu and W.J. Pitz. The International Combustion Symposium, Dublin, Ireland, July 30-August 3, 2018. https://doi.org/10.1016/j.proci.2018.06.097
- **An Ignition Delay and Chemical Kinetic Modeling Study of Prenol –** S. Wagnon, M. Mehl, W.J. Pitz, and H.J. Curran. 37th International Combustion Symposium, Dublin, Ireland, July 29-August 3, 2018.
- **An Overview of Caterpillar/Sandia Collaborative Research –** C. J. Mueller presented at Caterpillar Technical Center, Mossville, Illinois, May 3, 2018.

Publications & Presentations (5)

- **Annual Merit Review and Peer Review Evaluation Presentations –** 12 presentations: A. Agrawal, S. Curran, J. Farrell, G. Fioroni, C. Kolodziej, G. Lavoie, C. McEnally, M. McNenly, C. Mueller, J. Pihl, I. Schoegl, and S. Sluder. https://www.energy.gov/eere/vehicles/annual-merit-review-presentations
- **Autoignition of trans-Decalin, a Diesel Surrogate Compound: Rapid Compression Machine Experiments and Chemical Kinetic Modeling –** M. Wang, K. Zhang, G. Kukkadapu, S. W. Wagnon, M. Mehl, W. J. Pitz, and C.-J. Sung. Combustion and Flame, 194: 152-163, 2018. https://doi.org/10.1016/j.combustflame.2018.04.019
- **Bioconversion of Distillers' Grains Hydrolysates to Advanced Biofuels by an Escherichia Coli Co-Culture–** F. Liu, R.W. Davis, et al. Microbial Cell Factories, 16:192, 2017. https://doi.org/10.1186/s12934-017-0804-8
- **Bio-derived Building Blocks for Various Drop in Fuels and Value Added Chemicals** – O. Staples. Presented at the 255th American Chemical Society National Meeting, New Orleans, LA, March 18 -22, 2018.
- **Biomass Market Dynamics Supporting the Large-Scale Deployment of High-Octane Fuel Production in the United States—**P. Lamers, R.T. Nguyen, D.S. Hartley, J.K. Hansen, and E.M. Searcy. Global Change Biology: Bioenergy, April 2018. https://doi.org/10.1111/gcbb.12509
- **Breakout Technologies of Engine and Fuel** – D. Vuilleumier. Presented at the International Summit on International Scholar Exchange Fellowship 2018 at Tianjin University, China, August 20, 2018.
- **Chapter 17: Adding Value to the Biorefinery with Lignin: An Engineer's Perspective –** M. Biddy. RSC Energy and Environment Series, 19:499-518, January 2018. https://pubs.rsc.org/en/content/chapter/bk9781782625544-00499/978-1-78801-035-1
- **Co-Optima Initiative's Approach to Multimode Combustion –** J.P. Szybist presented at the SAE High Efficiency IC Engine Symposium, April 8, 2018. https://dx.doi.org/10.4271/04-11-03-0014
- **Co-Optimization of Fuels & Engines: Efficiency Merit Function for Spark Ignition Engines: Revisions and Improvements Based on FY16–17 Research and Development –** P.C. Miles. Technical Report DOE/GO-102018-5041, 2018. https://doi.org/10.2172/1463450

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- **Co-Optimization of Fuels & Engines: Fuel Blendstocks with the Potential to Optimize Future Gasoline Engine Performance; Identification of Five Chemical Families for Detailed Evaluation –** J.T. Farrell, J.E. Holladay, and R. Wagner. Technical Report, 1434413, April 2018. https://dx.doi.org/10.2172/1434413
- **Co-Optimization of Fuels & Engines: Properties of Co-Optima Core Research Gasolines –** R. McCormick, L.A. Fouts, G.M Fioroni, E.D. Christensen, M.A. Ratcliff, B.T. Zigler, S. Sluder, J.P. Szybist, S. Ciatti, J.T. Bays, W. Pitz, M. Mehl, J.E. Dec, and P.C. Miles. Technical Report 1467176, August 2018. https://dx.doi.org/10.2172/1467176
- **Combined Effects of Intake Flow and Spark-Plug Location on Flame Development, Combustion Stability and End-Gas Autoignition for Lean Spark-Ignition Engine Operation using E30 Fuel –** M. Sjöberg, and X. He. International Journal of Engine Research, 19(1):86-95, January 2018. https://doi.org/10.1177/1468087417740290
- **Combustion Characteristics of PRF and TSF Ethanol Blends in an Instrumented CFR Engine –** A. Hoth, C.P. Kolodziej, T. Rockstroh, and T. Wallner. SAE Technical Paper 2018-01-1672, 2018. https://doi.org/10.4271/2018-01-1672
- **Combustion Characteristics of Various Fuels during Research Octane Number Testing on an Instrumented CFR F1/F2 Engine –** C. Kolodziej and T. Wallner. Combustion Engines, 171(4):164-169, 2017. https://doi.org/10.19206/CE-2017-427
- **Compatibility Assessment of Fuel System Thermoplastics with Bio-Blendstock Fuel Candidates Using Hansen Solubility Analysis –** M. Kass, B. West. SAE Int. J. Fuels Lubr. 11(1):43-104, 2018 https://doi.org/10.4271/04-11-01-0004
- **Critical Fuel Property Evaluation for Potential Gasoline and Diesel Biofuel Blendstocks with Low Sample Volume Availability** – E. Polikarpov, K.O. Albrecht, J.P. Page, D. Malhotra, P. Koech, L. Cosimbescu, D.J. Gaspar. Fuel, September 24, 2018. https://doi.org/10.1016/j.fuel.2018.09.129
- **Demonstration of Fusel Alcohols as a Platform for a Tunable Suite of High Performance Biofuel Compounds for Advance Combustion Strategies –** E. Monroe, F. Liu, M. Tran-Gyamfi, A. George, and R. Davis. Oral presentation and Abstracts of Papers of The American Chemical Society, March 18, 2018.

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- **Development and Validation of a Chemical Kinetic Model for Diisobutylene, a High-Performance Fuel –** K. Zhang, M. Lailliau, Z. Serinyel, P. Dagaut, S. S. Matveev, G. Kim, B. Almansour, G. Dayma, A. Konnov, S. Vasu, and W. J. Pitz. Poster, 40th Task Leaders Meeting of the IEA Combustion Program, Fréjus, France, June 10-14, 2018.
- **Development and Validation of CFR Engine GT-Power Model for Estimating In-Cylinder Conditions –** S. Choi, A Hoth, C. Kolodziej, and T. Wallner. SAE Technical Paper 2018-01-0848, 2018. https://doi.org/10.4271/2018-01-0848
- **Development of a Cold Start Fuel Penalty Metric for Evaluating the Impact of Fuel Composition Changes on SI Engine Emissions Control –** J.A. Pihl, J.F. Thomas, S. S. Majumdar, S.P. Huff, B.H. West, and T.J. Toops. SAE Technical Paper 2018-01-1264, 2018. https://doi.org/10.4271/2018-01-1264
- **Development of a Virtual CFR Engine Model for Knocking Combustion Analysis –** P. Pal, C. Kolodziej, S. Choi, and S. Som et al. SAE Technical Paper 2018-01-0187. https://doi.org/10.4271/2018-01-0187
- **Discovery and Synthetic Demonstration of High-Performance Fuel via Solvent-Free Etherification –** N. Huq, X. Huo, J. Stunkel, P.C. St. John, S. Kim, R.L. McCormick, D.R. Vardon. ACS National Fall Conference, Boston, Massachusetts, August 2018.
- **Discovery of a RON Hyperboosting Phenomenon in Prenol/Gasoline Blends –** A. George. ACS National Fall Conference, Boston, Massachusetts, August 2018.
- **Ducted Fuel Injection: A New Approach for Lowering Soot Emissions from Direct-Injection Engines –** C.J. Mueller, C.W Nilsen, D.J. Ruth, R.K Gehmlich, L.M Pickett, and S.A. Skeen. WCX18: SAE World Congress Experience, Detroit, Michigan, April 11, 2018. https://www.osti.gov/biblio/1468317
- **Ducted Fuel Injection: A New Technology for Improving Engines and Fuels –** C. J. Mueller. Invited presentation for Medium-Duty and Heavy-Duty Vehicle Efficiency Opportunities through the Co-Optimization of Fuel and Engine Technologies panel discussion during WCX18: SAE World Congress Experience, Detroit, Michigan, April 10, 2018.
- **Effects of Fuel Laminar Flame Speed Compared to Engine Tumble Ratio, Ignition Energy, and Injection Strategy on Lean and EGR Dilute Spark Ignition Combustion –** C. Kolodziej, et al. SAE Technical Paper 2017-01-0671, April 2017. https://doi.org/10.4271/2017-01-0671

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- **Effects of Heat of Vaporization and Octane Sensitivity on Knock-Limited Spark Ignition Engine Performance –** M.A Ratcliff, J. Burton, P. Sindler, E. Christensen, L. Fouts, and R.L. McCormick. SAE Technical Paper 2018-01-0218, 2018. https://doi.org/10.4271/2018-01-0218
- **Effects of Increased Fuel Heat of Vaporization on the Research Octane Number Method** – C. Kolodziej, A. Hoth, T. Rockstroh, S. Choi, and T. Wallner. Oral-only presentation at SAE World Congress, Detroit, MI, April 10-12, 2018.
- **Effects of Pre-Spark Heat Release on Engine Knock Limit –** D. Splitter, A. Gilliam, J. Szybist and J. Ghandhi. Proc. Comb. Inst., available online June 2018. https://doi.org/10.1016/j.proci.2018.05.145
- **Engineering β-oxidation in Yarrowia Lipolytica for Methyl Ketone Production –** E. Hanko, C. Denby, V. Sànchez i Nogué, W. Lin, K. Ramirez, C. Singer, G. Beckham, and J. Keasling. Metabolic Engineering, 48:52-62, 2018. https://doi.org/10.1016/j.ymben.2018.05.018
- **Environmental, Economic, and Scalability Considerations and Trends of Selected Fuel Economy-Enhancing Biomass-Derived Blendstocks –** J.B Dunn, M. Biddy, S. Jones, H. Cai, P.T. Benavides, J. Markham, L. Tao, E. Tan, C. Kinchin, R. Davis, A. Dutta, M. Bearden, C. Clayton, S. Phillips, K. Rappe, and P. Lamers. ACS Sustainable Chemistry and Engineering, 6(1):561-569, 2017. https://pubs.acs.org/doi/abs/10.1021/acssuschemeng.7b02871
- **Estimation of the Fuel Efficiency Potential of Six Gasoline Blendstocks Identified by the U.S. Department of Energy's Co-Optimization of Fuels and Engines Program –** S. Sluder. AEC Program Review Meeting, Southfield, Michigan, August 14, 2018.
- **Ethanol Pyrolysis Kinetics Using H2O Time History Measurements Behind Reflected Shock Waves –** L.T. Pinzon, O. Mathieu, C. R. Mulvihill, I. Schoegl, and E.L. Petersen. Proc. Comb. Inst., available online August 2018. https://doi.org/10.1016/j.proci.2018.07.088
- **Experimental and Modeling Studies of a Biofuel Surrogate Compound: Laminar Burning Velocities and Jet-Stirred Reactor Measurements of Anisole –** S.W. Wagnon, S. Thion, E. J.K. Nilsson, M. Mehl, Z. Serinyel, K. Zhang, P. Dagaut, A.A. Konnov, G. Dayma, and W.J. Pitz, Combust. Flame, 189:325-336, March 2018. https://doi.org/10.1016/j.combustflame.2017.10.020

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- **Experimental and Modeling Study of Laminar Burning Velocities of Ethanol, N-propanol, Cyclopentanone and their Blends –** G. Capriolo, K. Zhang, G. Kim, B. Almansour, S.S. Vasu, W.J. Pitz, and A.A. Konnov. 37th International Combustion Symposium, Dublin, Ireland, July 29-August 3, 2018.
- **Experimental and Numerical Study of Variable Oxygen Index Effects on Soot Yield and Distribution in Laminar Co-flow Diffusion Flames –** A. Jain, D.D. Das, C.S. McEnally, L.D. Pfefferle, and Y. Xuan. Proc. Comb. Inst., available online June 2018. https://doi.org/10.1016/j.proci.2018.05.118
- **Experimental and Surrogate Modeling Study of Diesel Fuel –** G. Kukkadapu, R. Whitesides, M. Wang, SS Wagnon, K. Zhang, M. Mehl, W.J. Pitz, C.-J. Sung and C. Westbrook. 37th International Combustion Symposium, Dublin, Ireland, July 29-August 3, 2018.
- **Experimental and Theoretical Insight into the Soot Tendencies of the Methylcyclohexene Isomers –** S Kim, G. M. Fioroni, J. Park, D. J. Robichaud, D.D. Das, P.C. St. John, T. Lu, C.S. McEnally, L.D. Pfefferle, R.S. Paton, T.D. Foust, and R.L. McCormick. Proc. Comb. Inst., available online, July 2018. https://doi.org/10.1016/j.proci.2018.06.095
- **Experimental and Theoretical Study of Oxidative Stability of Alkylated Furans Used as Gasoline Blend Components –** E. Christensen, G.M. Fioroni, S. Kim, L. Fouts, E. Gjersing, R.S. Paton, and R.L. McCormick. Fuel, 212:576-585, January 2018. https://doi.org/10.1016/j.fuel.2017.10.066
- **Explicating Feature Contribution Using Random Forest Proximity Distances;** L.S. Whitmore, A. George, and C.M. Hudson; arXiv preprint arXiv:1807.06572
- **Exploring Bio-Derived Building Blocks For The Simultaneous Production of Fuels and Chemicals** – O. Staples. Presented at the 22nd American Chemical Society Green Chemistry & Engineering Conference in Portland, OR, June 18-20, 2018.
- **Exploring Gasoline Oxidation Chemistry in Jet Stirred Reactors Fuel –** B. Chen, Z. Wang, J. Wang, C. Togbe, P.E. Alonso, M. Almalki, H. Wang, M. Mehl, W.J. Pitz, S. Wagnon, K. Zhang, G. Kukkadapu, P. Dagaut, and M. Sarathy. Fuel, 236:1282-1292, September 2018. https://doi.org/10.1016/j.fuel.2018.09.055
- **Fuel Kinetic Effects on Pre-Spark Heat Release and Engine Knock Limit –** A. Gilliam, D.A. Splitter, J.P. Szybist, J. Ghandhi. Proceedings of THIESEL 2018 Conference on Thermo- and Fluid Dynamic Processes in Direct Injection Engines, September 2018. https://www.osti.gov/biblio/1468190

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- **Fuel Property Effect on Low-Speed Pre-Ignition –** G.S. Jatana, D.A. Splitter, B. Kaul, and J.P. Szbist. Fuel, 230:474-482, May 2018. https://doi.org/10.1016/j.fuel.2018.05.060
- **Fuel Property Prediction and Experimental Values –** D. Vardon presented at the American Chemical Society Green Chemistry Conference in Portland, Oregon, June 18-20, 2018.
- **Fuel-Film Thickness Measurements using Refractive Index Matching in a Stratified-Charge SI Engine Operated on E30 and Alkylate Fuels –** C.-P. Ding, M. Sjöberg, D. Vuilleumier, D.L. Reuss, X. He, and B. Böhm. Exp Fluids, 59:59, 2018. https://doi.org/10.1007/s00348-018-2512-5
- **Fueling Infrastructure Materials and Isobutanol Compatibility** – M. Kass and K. Moriarty. Webinar Presentation to the Steel Tank Institute, May 31, 2018.
- **Fuels and Combustion Research on the Argonne CFR F1/F2 Engine –** C. Kolodziej, T. Rockstroh, P. Pal, A. Hoth, S. Choi, S.S. Goldsborough, S. Som, T. Wallner, and M.C. Jespersen. ASTM D02 Meeting, Phoenix, Arizona, June 27, 2018.
- **Fungal Metabolites as Precursors to Renewable Transportation Fuels –** M.G. Butcher, P.A. Meyer, et al. Fuel, 215:123-141, March 2018. https://doi.org/10.1016/j.fuel.2017.10.052
- **Global Sensitivity Analysis (GSA) of Fuel Property Effects in Spark-Ignition (SI) Engines –** Z. Yue et al. AEC Program Review Meeting, Southfield, Michigan, August 14, 2018.
- **Green Gold? Supplanting Petroleum with Renewable Carbon** – A.D. Sutton. Invited presentation, Colorado State University, Inorganic Chemistry Seminar, Fort Collins, CO, October 17, 2017.
- **Impacts of Air-Fuel Stratification in ACI Combustion on Particulate Matter (PM) and Gaseous Emissions** – M. DeBusk presented data on the at the 2018 CLEERS workshop in Ann Arbor, Michigan, September 2018. https://cleers.org/wp-content/uploads/formidable/3/2018CLEERS_MelanieDeBusk_Poster_Web.pdf
- **Impact of Coolant Temperature on Piston Wall-Wetting and Smoke Generation in a Stratified-Charge DISI Engine Operated on E30 Fuel –** X. He, Y. Li, M. Sjöberg, D. Vuilleumier, C.-P. Ding, F. Liu, and X. Li. Proc. Comb. Inst., available online November 2018. https://doi.org/10.1016/j.proci.2018.07.073

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- **Impact of Engine Pressure-Temperature Trajectory on Autoignition for 19 Fuels: From Boosted SI (Beyond RON) to HCCI (Beyond MON) –** J.P. Szybist and D.A. Splitter. Presented to the AEC MOU, Southfield, Michigan, August 16, 2018.
- **Initiation of Flash Boiling of Multicomponent Miscible Mixtures with Application to Transportation Fuels and Their Surrogates –** C.T. Avedisian, K. Skyllingstad, R.C. Cavicchi, C. Lippe, and M.J. Carrier. Energy and Fuels, 32(9):9971-9981, September 2018. https://pubs.acs.org/doi/10.1021/acs.energyfuels.8b02258 **Insights into Engine Knock: Comparison of Knock Metrics across Ranges of Intake Temperature and Pressure in the CFR Engine –** T. Rockstroh, C.P. Kolodziej, M.C. Jespersen, S.S. Goldsborough, and T. Wallner. SAE Technical Paper 2018-01-0210, 2018. https://doi.org/10.4271/2018-01-0210
- **Introduction of Co-Optima Light-duty Multimode Engine Operation Research –** M. Sjöberg presented at the IEA Combustion Task Leaders Meeting in Frejus, France, June 12, 2018.
- **Investigation of the Impact of Fuel Properties on Particulate Number Emissions of a Modern Gasoline Direct Injection Engine –** M. Fatouraie, M. Frommherz, M. Mosburger, E. Chapman, S. Li, G.M. Fioroni, and R.L. McCormick. SAE Technical Paper 2018-01-0358, 2018. https://doi.org/10.4271/2018-01-0358
- **Investigation of the Spray and Combustion Characteristics of Four Multi-Component Diesel Surrogate Fuels Relative to their Commercial Target Fuel –** K. Yasutomi, C.J. Mueller, L.M. Pickett, and S.A. Skeen. THIESEL 2018: Conference on Thermo- and Fluid-Dynamic Processes in Direct Injection Engines, Valencia, Spain, September 12, 2018.
- **Isolating the Effects of Reactivity Stratification in Reactivity-Controlled Compression Ignition with Iso-Octane and N-Heptane on a Light-Duty Multi-Cylinder Engine –** M.L. Wissink, S.J. Curran, G. Roberts, M.P.B. Musculus, and C. Mounaïm-Rousselle. Int. J. of Eng. Res., 19:907-926, October 2017. https://doi.org/10.1177/1468087417732898
- **Kinetic Modeling of Ignition in Miniature Shock Tube –** M. Tao, P.T. Lynch, and P. Zhao. Proc. Comb. Inst., available online June 2018. https://doi.org/10.1016/j.proci.2018.05.048

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- **Kinetic Modeling Study of Surrogate Components for Gasoline, Jet and Diesel Fuels: C7-C11 Methylated Aromatics –** G. Kukkadapu, D. Kang, S.W. Wagnon, K. Zhang, M. Mehl, M. Monge-Palaciosc, H. Wang, S.S. Goldsborough, C.K. Westbrook, and W.J. Pitz. Proc. Combust. Inst., available online August 2018. doi: 10.1016/j.proci.2018.08.016
- **Large-Eddy Simulations of Spray Variability Effects on Flow Variability in a Direct-Injection Spark-Ignition Engine under Non-Combusting Operating Conditions –** N. Van Dam, M. Sjoberg, and S. Sibendu. SAE Technical Paper 2018-01-0196, 2018. https://doi.org/10.4271/2018-01-0196
- **Manifestation of Octane Rating, Fuel Sensitivity, and Composition Effects for Gasoline Surrogates Under Advanced Compression Ignition Conditions –** M. Tao, P. Zhao, D. DelVescovo, and H. Ge. Combust. Flame, 192:238-249, June 2018. https://doi.org/10.1016/j.combustflame.2018.02.015
- **Measured and Predicted Vapor Liquid Equilibrium of Ethanol-Gasoline Fuels with Insight on the Influence of Azeotrope Interactions on Aromatic Species Enrichment and Particulate Matter Formation in Spark Ignition Engines –** S. Burke, R. Rhoads, M. Ratcliff, R. McCormick, and B. Windom. SAE Technical Paper 2018-01-0361, 2018. https://doi.org/10.4271/2018-01-0361
- **Measurements and Prediction of Sooting Tendencies of Hydrocarbons and Oxygenated Hydrocarbons –** D. Das, P. St. John, C.S. McEnally, S. Kim and LD. Pfefferle. Presented at AIChE 2017, October 30, 2017.
- **Measuring and Predicting Sooting Tendencies of Oxygenates, Alkanes, Alkenes, Cycloalkanes, and Aromatics on a Unified Scale –** D.D. Das, P.C. St John, C.S. McEnally, S. Kim, and L.D. Pfefferle. Combust. Flame, 190:349-364, 2018. https://doi.org/10.1016/j.combustflame.2017.12.005
- **Micro Combustion of Primary Reference Fuels in Narrow Heated Channels –** V. Naralasetti. LSU Master's Theses, 4786, 2018. https://digitalcommons.lsu.edu/gradschool_theses/4786/
- **Multidimensional Numerical Simulations of Knocking Combustion in a Cooperative Fuel Research Engine –** P. Pal, Y. Wu, T. Lu, S. Som, et al. J. Energy Res. Technol, 2018. doi:10.1115/ICEF2017-3599
- **Multi-fuel Surrogate Chemical Kinetic Mechanisms for Real World Applications –** C.K. Westbrook, M. Mehl, W.J. Pitz, G. Kukkadapu, S. Wagnon and K. Zhang., Physical Chemistry Chemical Physics, 20:10588-10606, 2018. http://dx.doi.org/10.1039/C7CP07901J

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- **National Labs Examine Effects of New Fuels on Current Equipment –** M. Kass and K. Moriarty. PEI Journal, Second Quarter, 2018.
- **Near-azeotropic Volatility Behavior of Hydrous and Anhydrous Ethanol Gasoline Mixtures and Impact on Droplet Evaporation Dynamics –** B. Abdollahipoor, S.A. Shirazi, K.F. Reardon, and B.C. Windom. Fuel Processing Technology, 181:166-174, December 2018. https://doi.org/10.1016/j.fuproc.2018.09.019
- **Next Generation Biofuel Production –** C.M. Moore, Invited presentation, Department of Chemistry and Biochemistry, University of San Diego, San Diego, CA, July 18, 2018.
- **Numerical Investigation of Central Fuel Property Hypothesis Using Virtual CFR Engine Model –** P. Pal et al. AEC Program Review Meeting, Southfield, Michigan, August 14, 2018.
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