DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Co-Optima Overview

March 15, 2021

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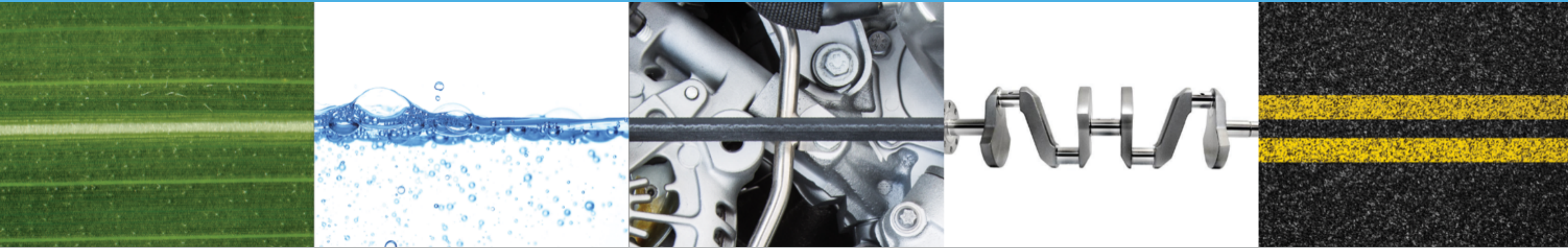
Pacific Northwest National Laboratory

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



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

Project Overview

Goal

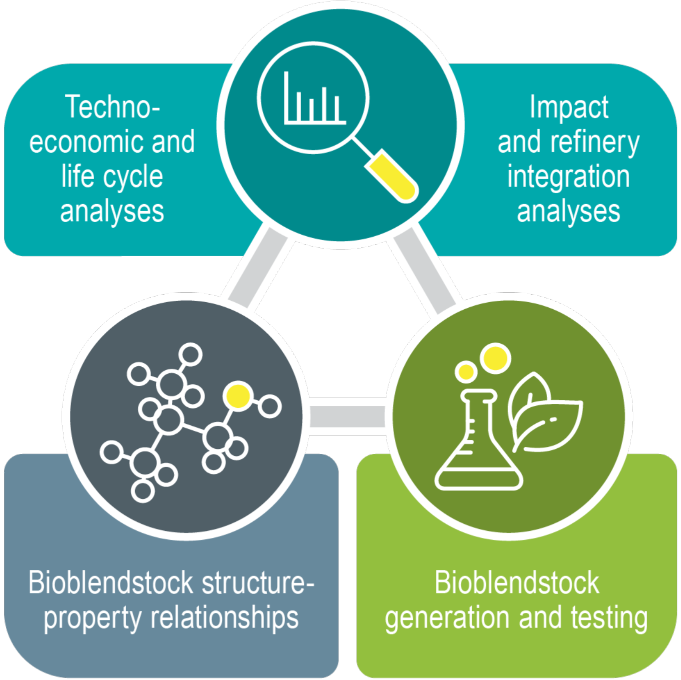
Identify low carbon fuel-engine combinations that increase fuel economy by 35% (light duty) or 4% (heavy duty) with reduced emissions over 2015 baseline.

Outcome

Definition of critical fuel properties that maximize performance, bio-blendstocks that provide target values of these properties and impacts of adoption–reducing emissions and providing economic benefits.

Relevance

Addresses BETO goal to enhance the bioenergy value proposition and increase market pull.



Techno-economic and life cycle analyses

Impact and refinery integration analyses

Bioblendstock structure-property relationships

Bioblendstock generation and testing

Project Overview

Provide technology options to increase sustainability of transportation

Light Duty

- 10% fuel economy gain over 2015 baseline

Medium- and Heavy-Duty

- Lower-cost path to reduced engine-out criteria emissions
- Up to 4% fuel economy gain

Biofuels

- Increase market opportunities for biofuels
- Diversify resource base
- Provide economic options to fuel providers to accommodate changing demands and drivers

Crosscutting Goals

- Decrease GHGs by at least 20% in the near term for 30% renewable blends
- Stimulate domestic economy and decrease petroleum imports
- Increase clean energy options and add new bio-economy jobs

Project Overview

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Techno-economic and life cycle analyses

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Crosscutting Goals

Techno-economic and life cycle analyses

Impact and refinery integration analyses

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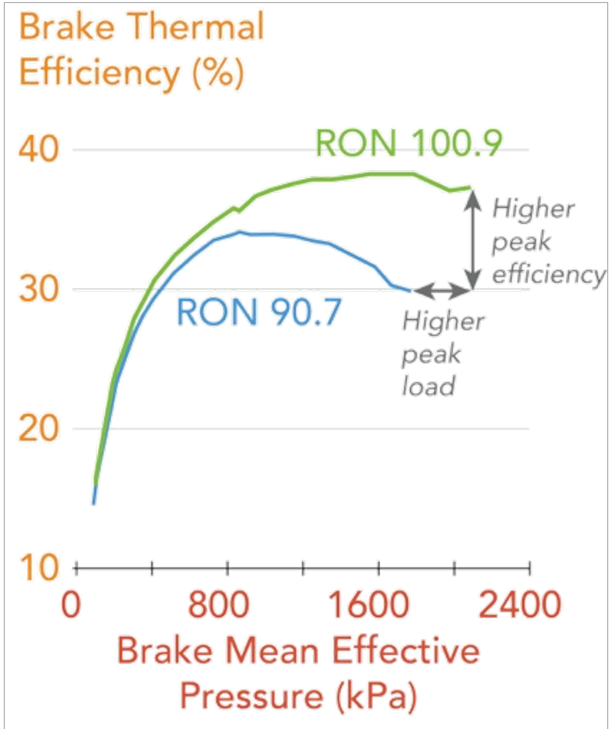
Project Overview – Motivation

Today's engines do not operate at peak efficiency…

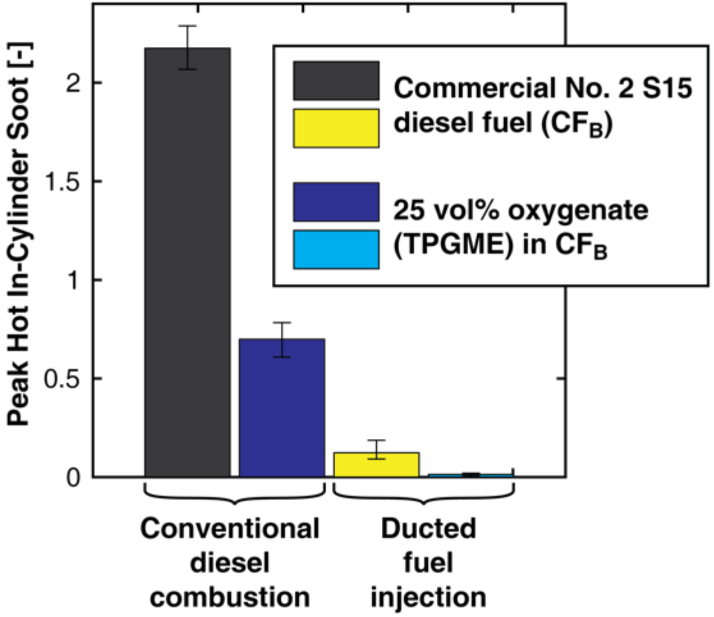


Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR source: C.S. Sluder, ORNL

- IC engines do not operate at peak efficiency with minimum emissions
- Changing fuel properties, engine and emissions system can improve performance
- Co-Optima focuses on understanding:
  - Fuel chemistry
  - Fuel properties
  - Benefits of sustainable production, use

Project Overview – Motivation

…with minimum emissions



Low-sooting blendstocks and new engine technology can reduce soot production by >98%

- IC engines do not operate at peak efficiency with minimum emissions
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- Co-Optima focuses on understanding:
  - Fuel chemistry
  - Fuel properties
  - Benefits of sustainable production, use

1. Management

1. Management

Organized to maintain input and oversight from DOE and stakeholders

Board of Directors
(Labs and DOE)

Approve direction, changes

Steering Committee

POC for each lab, communications, IP

Leadership Team
(Labs and DOE)

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

External Advisory Board

Advise on technology and direction, provide recommendations, serve as bridge to stakeholders

Project Manager

Monitor project plan and track milestones

Technical Team Leads

Plan and execute tasks, report monthly highlights and quarterly progress

1. Management

Teamwork drives technical achievements of national lab staff and collaborators

- Participating laboratories include Argonne, Idaho, Lawrence Berkeley, Lawrence Livermore, Los Alamos, National Renewable Energy Lab, Oak Ridge, Pacific Northwest, and Sandia National Laboratories
- University and industry collaborators funded via FOAs, DFOs

1. Management

Senior leadership at DOE and member Labs provide strong oversight and guidance

Board of Directors

DOE

- Michael Berube (Acting Dep Asst Secretary, EERE)
- Valerie Reed (Acting BETO Director)
- Dave Howell (VTO Director)

Labs (Assoc. Lab Directors)

- Johney Green (NREL)
- Xin Sun (ORNL)
- Jud Virden (PNNL)
- Andy McIlroy (SNL)

Leadership Team

DOE

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

Labs

- Dan Gaspar, Lead (PNNL)
- Bob McCormick (NREL)
- Robert Wagner (ORNL)
- Anthe George (SNL)

1. Management

External advisory board provides candid input from full range of stakeholders

Responsibilities

1. Provide recommendations on opportunities and future direction of Co-Optima
2. Meet in-person two times a year and by phone two times a year
3. Stay abreast of Co-Optima developments (e.g., through dialing into Monthly Stakeholder calls)
4. Support outreach to other organizations

Membership

- David Foster (chair)
  Professor (emeritus), University of Wisconsin
- Steve Berry
  Engine Manufacturers Association
- Ralph Cavalieri
  Professor (emeritus), Washington State University
- John Eichberger
  Fuels Institute
- Laurel Harmon
  LanzaTech
- Paul Machiele
  U.S. Environmental Protection Agency
- Danielle Magadia
  California Air Resources Board
- Scott Mason
  American Petroleum Institute and Phillips 66
- Paul Najt
  U.S. Council for Automotive Research (USCAR) and General Motors
- Ian Purtle
  Cargill (retired)
- John Wall
  Cummins (retired)
- Edgar Wolff-Klammer
  Underwriters Laboratory

1. Management

Ongoing input and outreach to broad range of stakeholders

Stakeholder "Listening Days"

Direct outreach visits

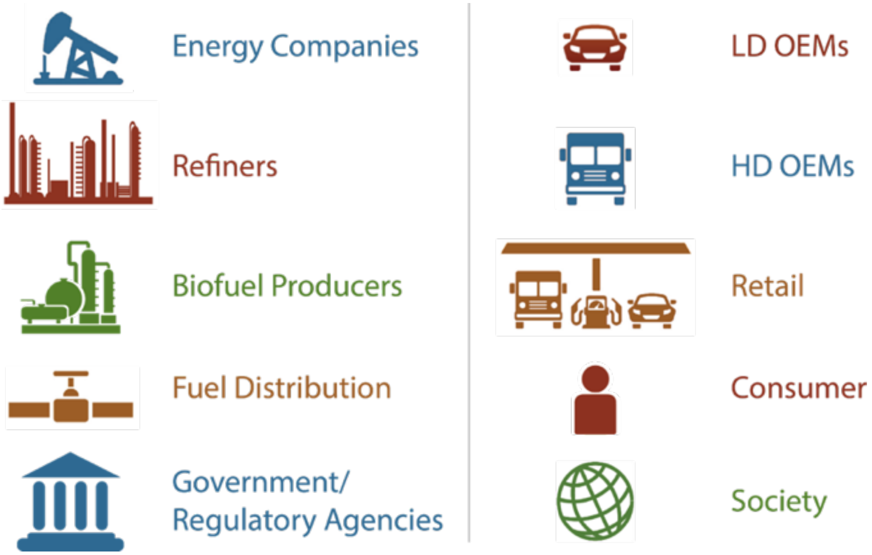
- >60 visits to OEMs, fuel providers, retail, biofuel companies, etc.
- Virtual updates

Interactive forums through technical societies

Monthly webinars

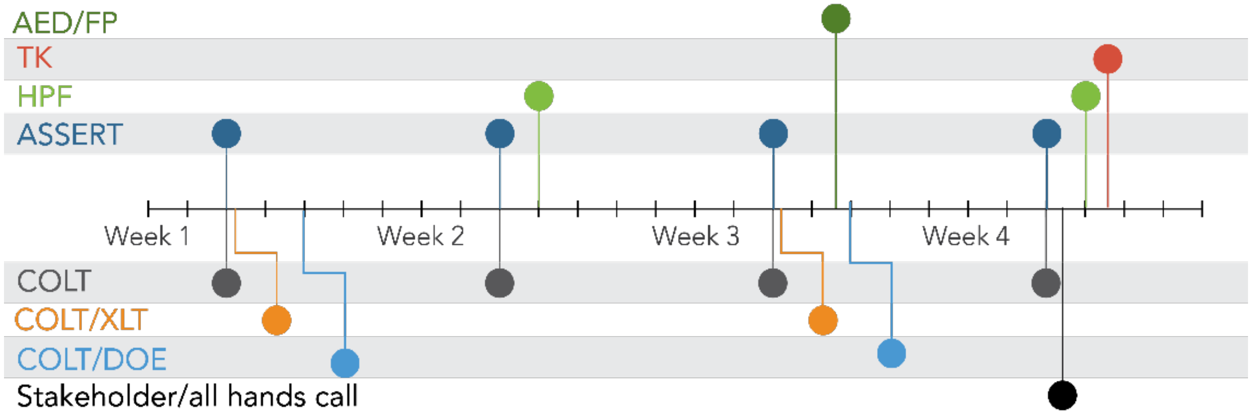
- 145 individuals
- 86 organizations

VTO Annual Merit Review and BETO Peer Review

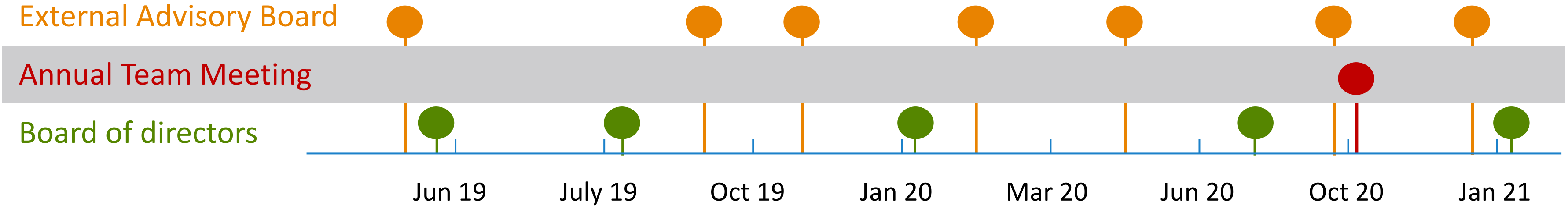


1. Management

Regular internal and stakeholder updates produce information flow



AED = Adv Engine Dev Team
ASSERT = Analysis of Sustainability, Scale, Economics, Risk and Trade Team
FP = Fuel Properties Team
HPF = High Performance Fuels Team
TK = Simulation Toolkit Team
COLT = Co-Optima Leadership Team
XLT = Extended Leadership Team



1. Management

Co-Optima approach designed to mitigate technology adoption risk

Co-Optima Major Risk Factors	Risk Mitigation Strategy
ICEs may be overtaken by electrification	Shift effort to MD/HD, focus on LD transition
Early-stage research difficult to de-risk for adoption, uptake by industry	Outreach to industry, other stakeholders, and research to address barriers
Feedstock supply, cost and production capacity required for market adoption	Leverage BETO program models and results on feedstocks, production
Large uncertainties around GHG reduction estimates for pre-pilot research	Use standard tools and approaches and benchmark against certified pathways

2. Approach

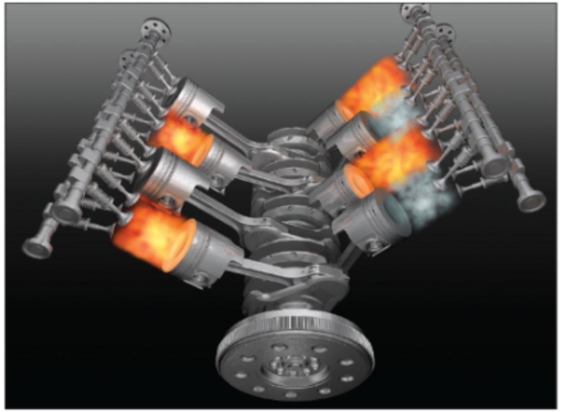
2. Approach

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

Research spans on-road from light-duty to heavy-duty

Light-Duty

- **Near-term - LD boosted SI combustion** opportunity with improved efficiency at higher load.
- **Longer-term - LD multi-mode combustion** includes boosted SI and ACI,* opportunity through improved efficiency *across* the drive-cycle.

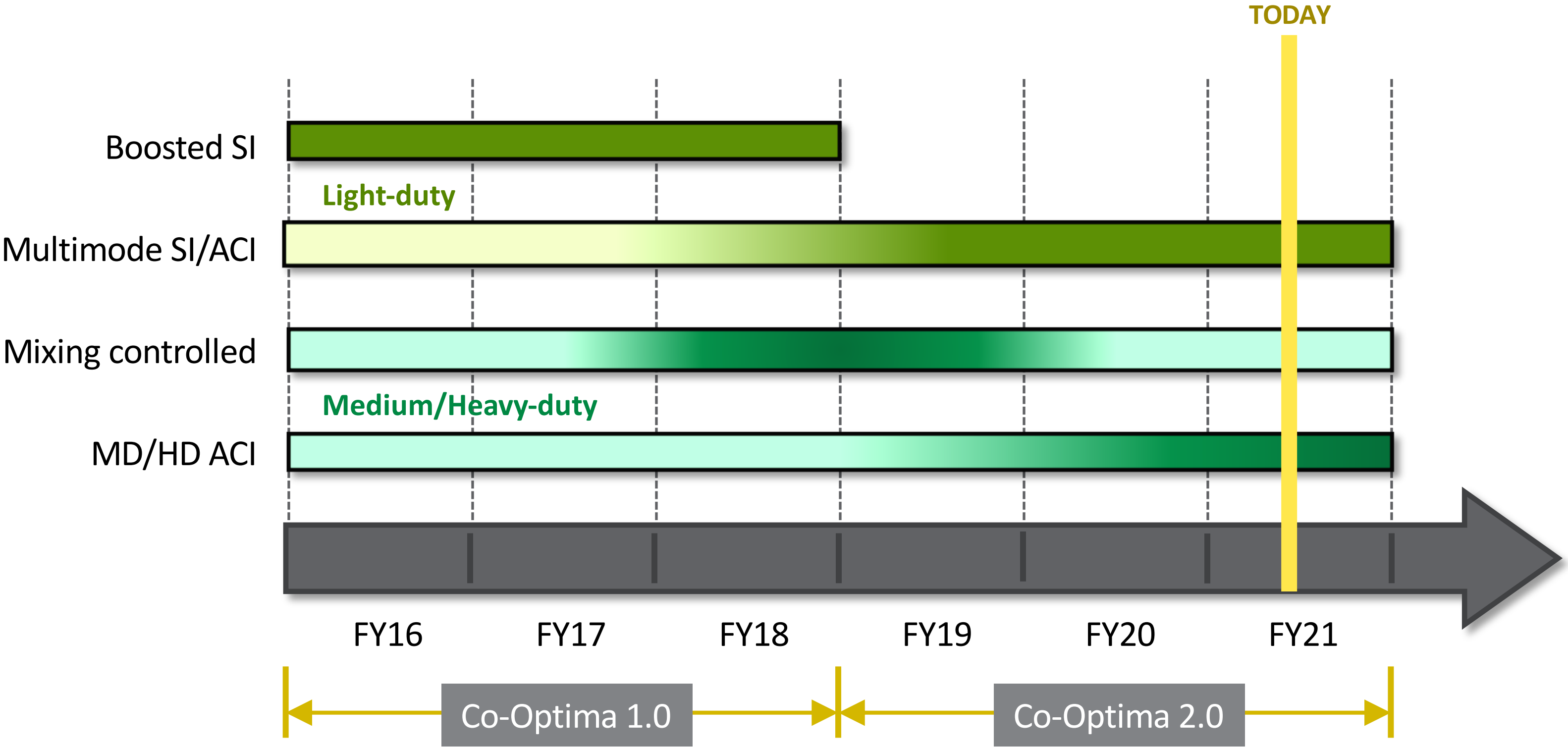
Medium/Heavy-Duty

- **Near-term - MD/HD MCCI**** with more conventional diesel combustion strategies.
- **Longer-term - MD/HD ACI** opportunity for improved low-load emissions and efficiency including multi-mode solutions.

*ACI – Advanced Compression Ignition
**MCCI – Mixing Controlled Compression Ignition

2. Approach

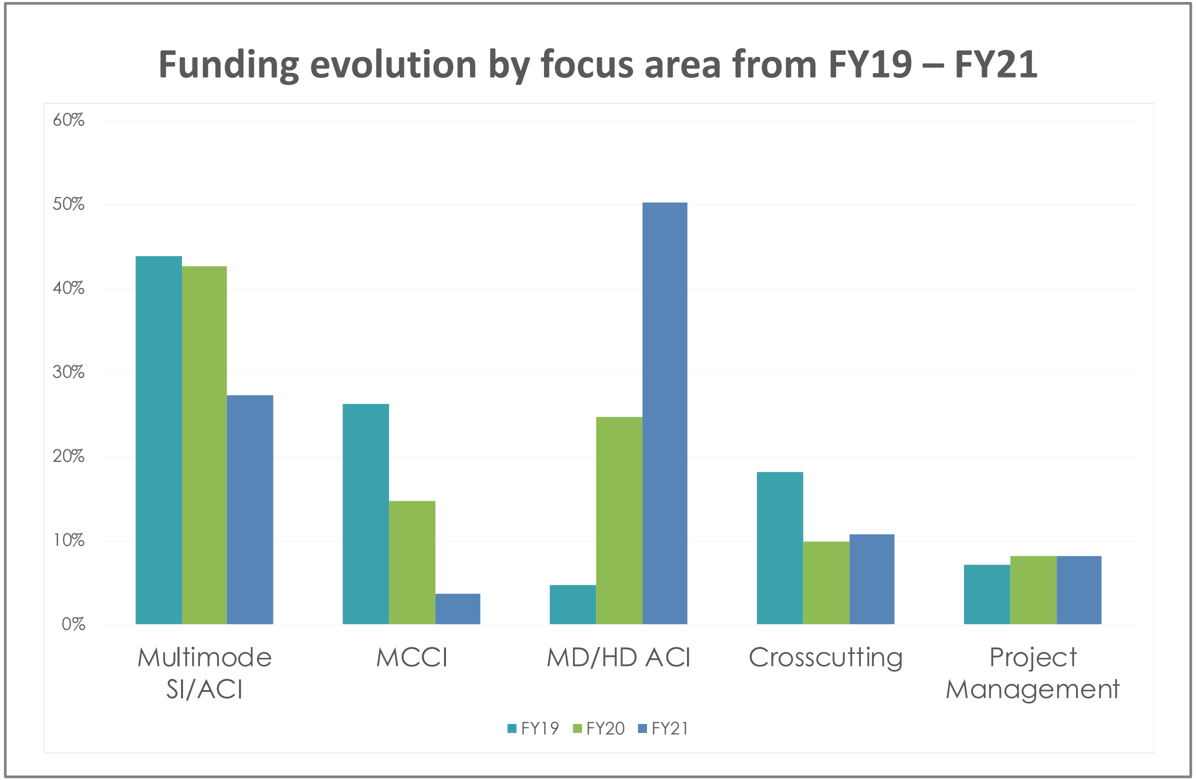
Activities staged to address near-term and longer-term opportunities



2. Approach

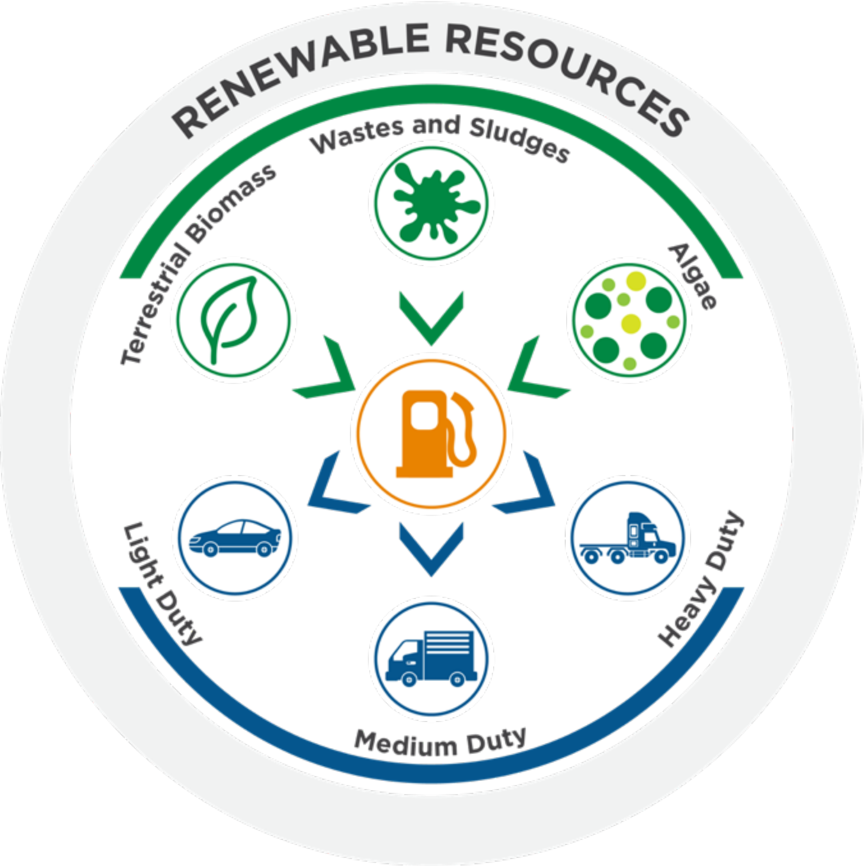
FY21 research funding illustrates continued shift to MD and HD

- 103 tasks funded by DOE VTO and BETO in FY2021 and are underway



2. Approach

Co-Optima activities evaluate sustainable fuel search space with key constraints



- Focus only on liquid fuels
- Identify blendstocks to blend into base fuel
- Consider only non-food-based biofuel feedstocks
- Assess well-to-wheels impacts for biofuel options (GHG, etc.)
- Provide data, tools, and knowledge to stakeholders – not “picking winners”

2. Approach

Milestones roll up to high-level objectives used to ensure tasks are aligned

	FY 2019 Q1-Q2	FY 2019 Q3-Q4	FY 2020 Q1-Q2	FY 2020 Q3-Q4	FY 2021 Q1-Q2	FY 2021 Q3-Q4
MM			A – Quantify relationships between fuel properties and engine parameters for combustion approaches (Sjoberg, Szybist)	B – Determine target values of critical fuel properties and ranges for each combustion approach (Szybist) C – Provide a list of blendstocks that provide key fuel properties (George) Blendstock Feasibility Go/No-Go (Q2 FY20, ANL)	D – Provide TEA, LCA, and refinery benefits analysis for candidate blendstocks (Hawkins) G – Identify/develop a fuel property metric to capture fuel autoignition behavior under ACI conditions relevant to SI/ACI multimode engines (Kolodziej)	F – Assess fuel property impacts on engine efficiency and fuel economy and emissions (Sjoberg) E – Provide transportation sector-level analyses indicating potential for impact at scale (Hawkins) H – Identify a pathway to emissions compliance (or potential aftertreatment architectures?) for a multimode SI/ACI engine (Pihl)
MCCI	B – Create and populate a merit table that links fuel properties to MCCI engine characteristics C – Determine target values of fuel properties for MCCI	A – Assessment of fuel property impacts on ducted fuel injection (DFI) technology to reduce emissions (Mueller)	D – Provide a list of MCCI blendstocks that provide key fuel properties [when blended with diesel] (George) G – Experimental confirmation of NO_x and PM reduction potential and other key characteristics of promising MCCI blendstocks (McCormick)		E – Provide TEA, LCA, and refinery benefits analysis for candidate MCCI blendstocks (Hawkins)	F – Transportation sector-level analyses indicating potential for impact at scale; determine if electrification of diesel vehicles can provide additional benefits, assess the expected fuel economy gains, and provide estimates of other factors (Hawkins)
MD/HD ACI				A – Determine target values of fuel properties and ranges for each combustion approach (Dec, Kolodziej) *Shifted from Q2 to Q3*		B – Demonstrate how alternative HPF blendstocks can be used to tailor a gasoline-range fuel that provides enhanced combustion-phasing control in MD/HD ACI engines while maintaining low NO_x and PM. (Dec) C – Determine the potential for diesel-range fuel properties (e.g., reduced boiling range) to enable low-load ACI operation in a MD/HD engine with ultra-low engine-out NO_x emissions under conditions where exhaust temperatures are too low to reduce engine-out NO_x with current emissions controls technologies. (Curran) D – Provide a list of blendstocks that provide key fuel properties (George)

Planned high level outcomes for Co-Optima 2.0 (FY19-FY21) are on track

2. Approach

FY21 objectives aim to complete MM, MCCI and finish experiments for MD/HD ACI

	FY 2021, Q1-Q2	**FY 2021,** Q3-Q4
Multimode	D – Provide TEA, LCA, and refinery benefits analysis for candidate blendstocks (Hawkins) G – Identify/develop a fuel property metric to capture fuel autoignition behavior under ACI conditions relevant to SI/ACI multimode engines (Kolodziej)	F – Assess fuel property impacts on engine efficiency and fuel economy and emissions (Sjoberg) E – Provide transportation sector-level analyses indicating potential for impact at scale (Hawkins) H – Identify a pathway to emissions compliance (or potential aftertreatment architectures) for a multimode SI/ACI engine (Pihl)
Mixing Controlled	E – Provide TEA, LCA, and refinery benefits analysis for candidate MCCI blendstocks (Hawkins)	F – Transportation sector-level analyses indicating potential for impact at scale; determine if electrification of diesel vehicles can provide additional benefits, assess the expected fuel economy gains, and provide estimates of other factors (Hawkins)
MD/HD ACI		B – Demonstrate how alternative HPF blendstocks can be used to tailor a gasoline-range fuel that provides enhanced combustion-phasing control in MD/HD ACI engines while maintaining low NO_x and PM. (Dec) C – Determine the potential for diesel-range fuel properties (e.g., reduced boiling range) to enable low-load ACI operation in a MD/HD engine with ultra-low engine-out NO_x emissions under conditions where exhaust temperatures are too low to reduce engine-out NO_x with current emissions controls technologies. (Curran) D – Provide a list of blendstocks that provide key fuel properties (George)

2. Approach

FY2020 Go/No Go successfully completed

Identify at least three bio-blendstocks that:

- exhibit target fuel properties values in support of efficient and clean **multimode** combustion while
- meeting advanced biofuel criteria, including at least 60% reduction in lifecycle carbon emissions, and
- volumetric cost-performance parity with petroleum reformate.

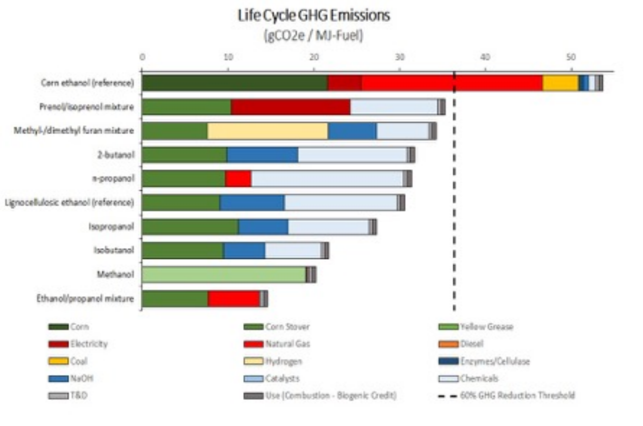
	Property/Metric	1-BuOH	i-PrOH	Furan mixture	i-BuOH	EtOH
Fuel Properties	MON (>84)	85	97	87	93	90
	RON (>98)	98	113	102	107	109
	S, RON-MON (>10)	13	16	15	14	19
	Blending Performance	Linear or mildly Syn.	Syn.	Syn.	Syn.	Syn.
	Volumetric Blending RON[#] (>95)	101	123	147	117	142
	Volumetric Blending S[#] (>10)	11	18	38	19	30
GHG	Global warming potential, gCO2-eq./MJ	31	27	34	22	31
	% reduction from conventional gasoline (>60%)	66%	70%	62%	76%	66%
Cost	Minimum Fuel Sale Price, USD/gge	$2.45	$4.33	$3.80	$3.71	$3.84
	Equivalent Volume Ratio relative to Petroleum Reformate (RON=102)[!]	1.08	0.40	0.24	0.48	0.26

2. Approach

Completed regular and dashboard milestones

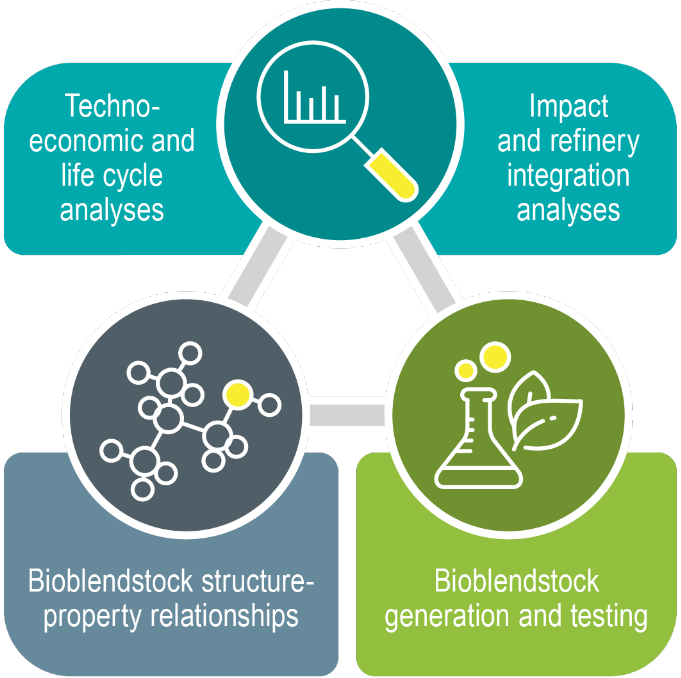
- Completed BETO milestones
    - FY19 – 38
    - FY20 – 34 with 14 more delayed due to COVID
- Completed 8 high-level objectives in FY19-20
- Completed 4 dashboard milestones aimed at identifying performance-advantaged MM blendstocks

Finalize list of at least 8 bioblendstocks that can enable multimode combustion while meeting advanced biofuel carbon emissions targets determined by LCA, which have high market potential established by TEA, and have demonstrated synergistic blending performance for critical fuel properties.	**Production and performance metrics**	**9/30/20**	**Annual Milestone (Regular)**



2. Approach

Co-Optima tasks coordinated to achieve research aims

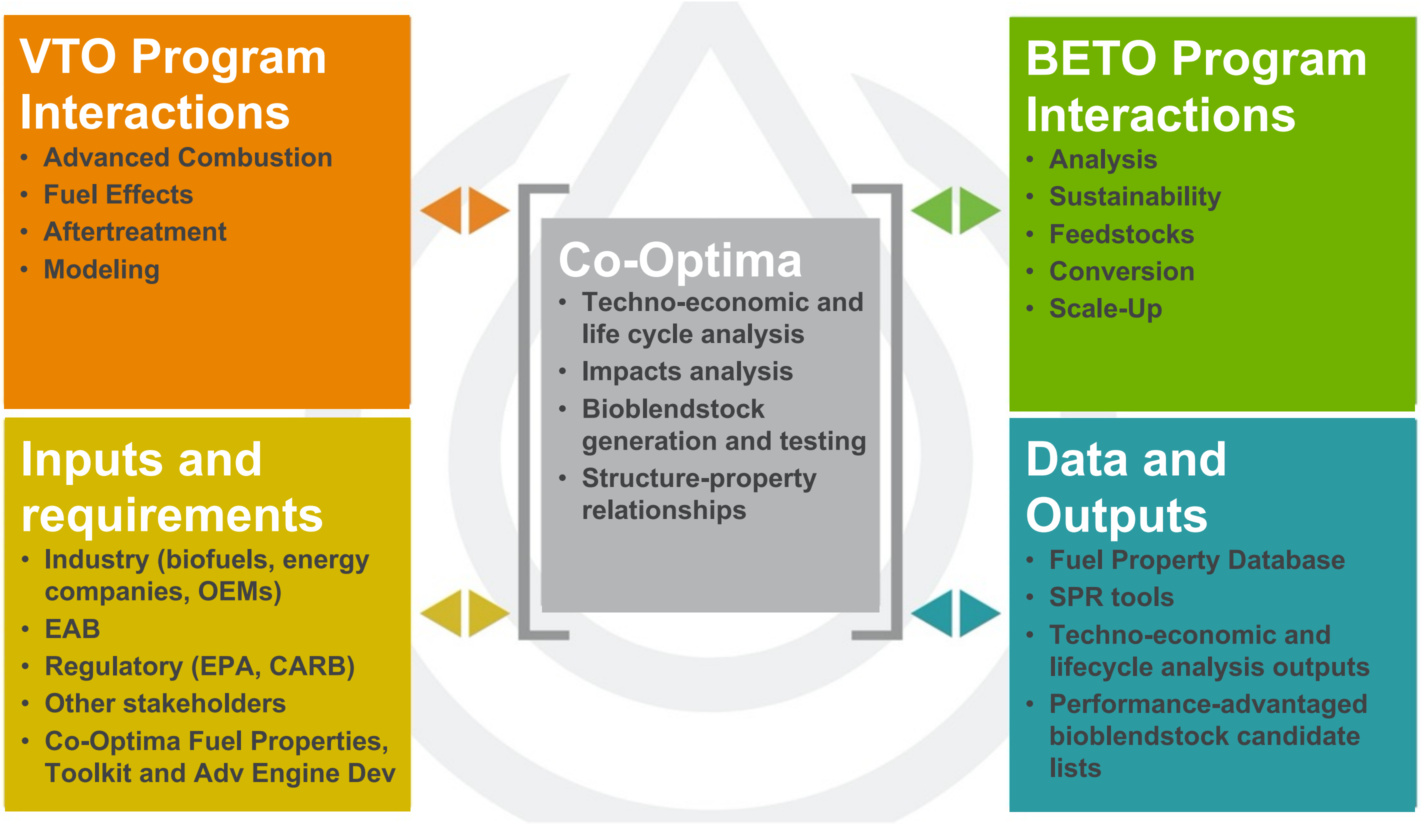


- Input from external sources, VTO-funded teams drives fuel property targets
- Fuel property data, computation and experiment used to develop and exploit structure-property relationships
- TEA and LCA inform bioblendstock identification throughout process
- Analysis of impacts informs further bioblendstock identification and testing

3. Impact

3. Impact

Co-Optima connects with stakeholders, and the broader BETO and VTO programs



VTO Program Interactions

- Advanced Combustion
- Fuel Effects
- Aftertreatment
- Modeling

Inputs and requirements

- Industry (biofuels, energy companies, OEMs)
- EAB
- Regulatory (EPA, CARB)
- Other stakeholders
- Co-Optima Fuel Properties, Toolkit and Adv Engine Dev

Co-Optima

- Techno-economic and life cycle analysis
- Impacts analysis
- Bioblendstock generation and testing
- Structure-property relationships

BETO Program Interactions

- Analysis
- Sustainability
- Feedstocks
- Conversion
- Scale-Up

Data and Outputs

- Fuel Property Database
- SPR tools
- Techno-economic and lifecycle analysis outputs
- Performance-advantaged bioblendstock candidate lists

3. Impact

Increased industry interest in performance-advantaged blendstocks and analyses

Panel discussions with industry, government, and university experts at annual meeting

- DOE
- Pepsico
- Cummins
- Chevron
- Shell
- Aachen Univ. Fuel Science Center
- Georgia Tech
- UC-Davis
- National Biodiesel Board

Recent and upcoming outreach

- Coordinating Research Council Advanced Vehicle Fuel and Lubricants Committee
- National Ethanol Conference/ RFA
- Cummins
- Manufacturers of Emission Controls Association
- Phillips 66
- CARB
- National Biodiesel Board
- CONCAWE
- 21st Century Truck Partnership

3. Impact

Industry response to FY2020 and FY2021 DFOs demonstrates relevance

Directed Funding Opportunity

- Co-Optima seeks proposals to leverage *national laboratory resources* to overcome key technical challenges.
- Projects aimed at specific technical challenges that Co-Optima researchers can help address to move biofuels closer to market for advanced, high-efficiency engines.

FY2020 DFO

- $200K-$300K per award
- 7 awards
- 12-18 month duration
- 20% cost share required
- $2M total, BETO

DFO capabilities matrix

https://cooptima.org/capabilities/

Awards announced July 3, 2020

FY2021 DFO

- $250K per award
- 4 awards expected
- 12-18 month duration
- 20% cost share required
- $1M total, BETO and VTO

DFO capabilities matrix

https://cooptima.org/capabilities/

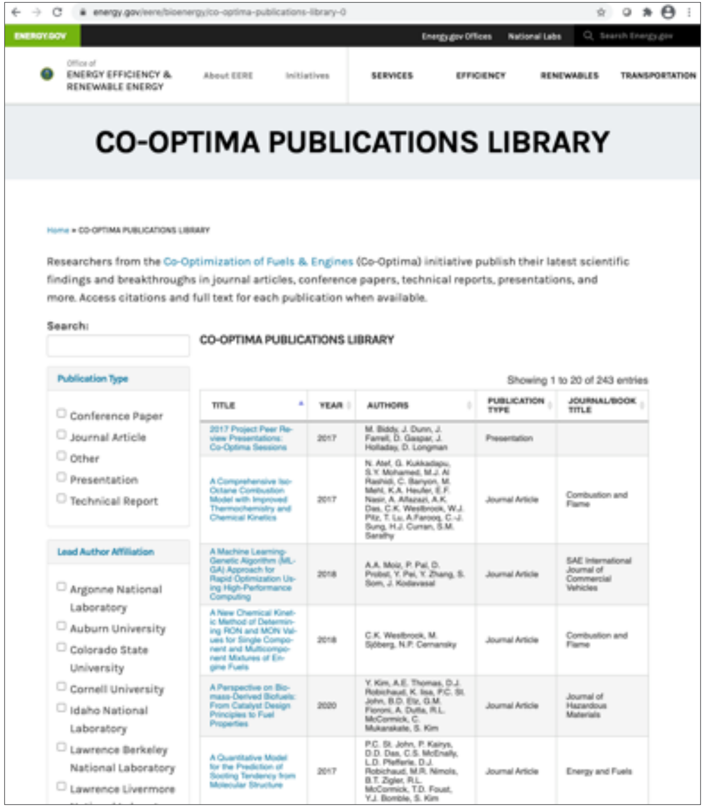
17 proposals received

3. Impact

Number of publications and patents continues to increase

Since FY19

- 123 publications
- 6 patents granted
- Publications on database among most viewed and most downloaded sites on BETO website



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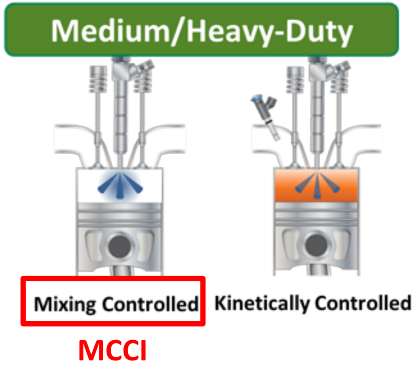
Showing 1 to 20 of 243 entries

TITLE	YEAR	AUTHORS	PUBLICATION TYPE	JOURNAL/BOOK TITLE
2017 Project Peer Review Presentations: Co-Optima Sessions	2017	M. Biddy, J. Dunn, J. Farrell, D. Gaspar, J. Holladay, D. Longman	Presentation	
A Comprehensive Iso-Octane Combustion Model with Improved Thermochemistry and Chemical Kinetics	2017	N. Atef, G. Kukkadapu, S.Y. Mohamed, M.J. Al Rashidi, C. Banyon, M. Mehl, K.A. Heufer, E.F. Nasir, A. Alfazazi, A.K. Das, C.K. Westbrook, W.J. Pitz, T. Lu, A.Farooq, C.-J. Sung, H.J. Curran, S.M. Sarathy	Journal Article	Combustion and Flame
A Machine Learning-Genetic Algorithm (ML-GA) Approach for Rapid Optimization Using High-Performance Computing	2018	A.A. Moiz, P. Pal, D. Probst, Y. Pei, Y. Zhang, S. Som, J. Kodavasal	Journal Article	SAE International Journal of Commercial Vehicles
A New Chemical Kinetic Method of Determining RON and MON Values for Single Component and Multicomponent Mixtures of Engine Fuels	2018	C.K. Westbrook, M. Sjöberg, N.P. Cernansky	Journal Article	Combustion and Flame
A Perspective on Biomass-Derived Biofuels: From Catalyst Design Principles to Fuel Properties	2020	Y. Kim, A.E. Thomas, D.J. Robichaud, K. Iisa, P.C. St. John, B.D. Etz, G.M. Fioroni, A. Dutta, R.L. McCormick, C. Mukarakate, S. Kim	Journal Article	Journal of Hazardous Materials
A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure	2017	P.C. St. John, P. Kairys, D.D. Das, C.S. McEnally, L.D. Pfefferle, D.J. Robichaud, M.R. Nimlos, B.T. Zigler, R.L. McCormick, T.D. Foust, Y.J. Bomble, S. Kim	Journal Article	Energy and Fuels

4. Progress and Outcomes

4. Progress and Outcomes

Identified target chemistries to meet Co-Optima goals



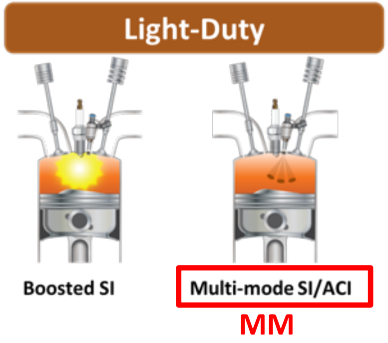
Performance:

CN, Sooting,

Flash point, LHV

Operability:

M_{p}, η, solubility, stability



Performance:

RON, MON, S, phi-sensitivity, HoV, Sooting

Operability:

P_{vap}, B_{p}, M_{p}, η, σ, stability

Light Duty: moved from SI to MM　　Medium/Heavy Duty: Accelerated MCCI effort

4. Progress and Outcomes

Produced and tested blendstocks to screen candidates, identify barriers

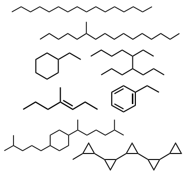
Biomass & Waste Carbon

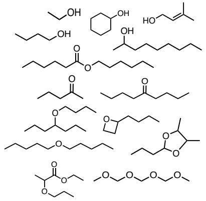
Direct Biological

Thermo/Chemical

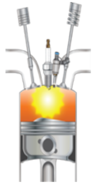
Hybrid Processes

Hydrocarbons & Oxygenates





Light & Heavy-Duty Fuels



Light Duty

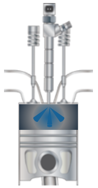
RON / MON / S

Energy Density

Flash / Boil / Freeze

RVP / HOV

Sooting



Heavy Duty

Cetane

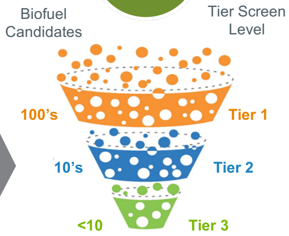
Energy Density

Flash / Boil / Freeze

Water Sol

Sooting

Tiered Testing & Analysis



Techno-Economic & Lifecycle Analysis

Scale from mL to multi-L

10 mL Fuel Property Screen

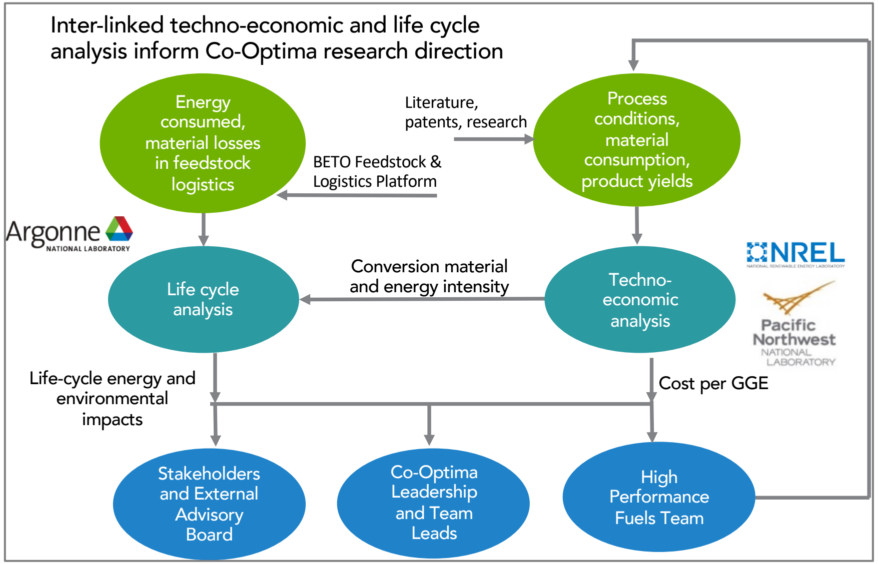
100 mL Tiered Screening Tests

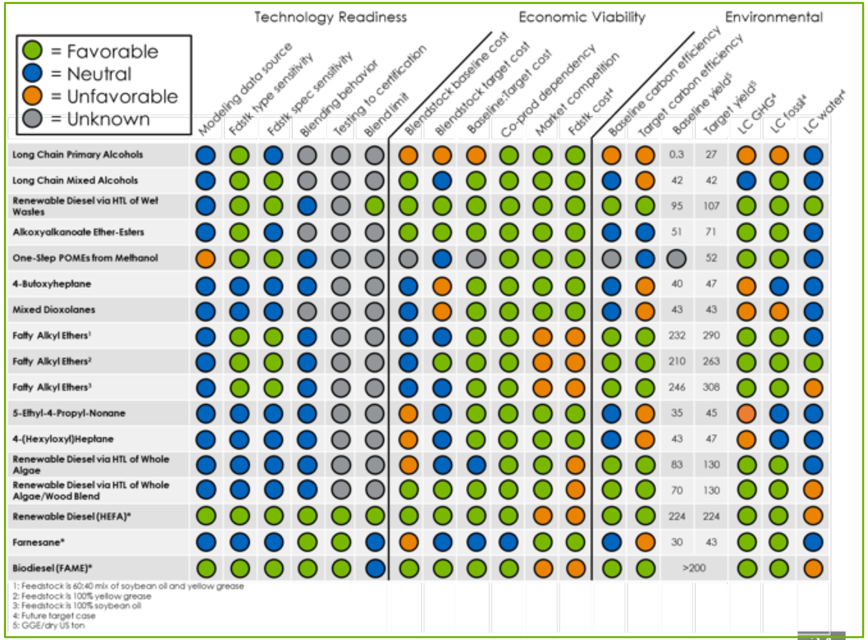
1 Liter Polymer & Single Cylinder

Multi-Liter Engine Testing

4. Progress and Outcomes

Techno-economic and life cycle analyses refined candidate lists, identified barriers


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



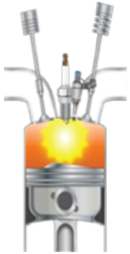
🟢 = Favorable
🔵 = Neutral
🟠 = Unfavorable
⚪ = Unknown

	Technology Readiness						Economic Viability						Environmental						
	Modeling data source	Fdstk type sensitivity	Fdstk spec sensitivity	Blending behavior	Testing to certification	Blend limit	Blendstock baseline cost	Blendstock target cost	Baseline:Target cost	Co-prod dependency	Market competition	Fdstk cost⁴	Baseline carbon efficiency	Target carbon efficiency	Baseline yield⁵	Target yield⁵	LC GHG⁴	LC fossil⁴	LC water⁴
Long Chain Primary Alcohols	🔵	🟢	🔵	⚪	⚪	⚪	🟠	🟠	🟠	🟢	🟢	🟢	🟠	🟠	0.3	27	🟠	🟠	🔵
Long Chain Mixed Alcohols	🔵	🟢	🟢	⚪	⚪	⚪	🟢	🔵	🟢	🟢	🟢	🟢	🔵	🟠	42	42	🔵	🟢	🔵
Renewable Diesel via HTL of Wet Wastes	🔵	🟢	🟢	🔵	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	95	107	🟢	🟢	🟢
Alkoxyalkanoate Ether-Esters	🔵	🟢	🔵	⚪	⚪	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🔵	🔵	51	71	🟢	🟢	🔵
One-Step POMEs from Methanol	🟠	🟢	🟢	🔵	⚪	⚪	⚪	🔵	⚪	🟢	🟢	🟢	⚪	🔵	⚪	52	🟢	🟢	🔵
4-Butoxyheptane	🔵	🔵	🔵	🔵	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	40	47	🟠	🔵	🔵
Mixed Dioxolanes	🔵	🔵	🔵	⚪	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	43	43	🟠	🟠	🔵
Fatty Alkyl Ethers¹	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	232	290	🟢	🟢	🔵
Fatty Alkyl Ethers²	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🟢	🟢	🟢	🟠	🟠	🟢	🟢	210	263	🟢	🟢	🟢
Fatty Alkyl Ethers³	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	246	308	🟢	🟢	🟠
5-Ethyl-4-Propyl-Nonane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟠	35	45	🟠	🔵	🔵
4-(Hexyloxyl)Heptane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟠	43	47	🟠	🔵	🔵
Renewable Diesel via HTL of Whole Algae	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🔵	🟢	🟢	🟠	🟢	🟢	83	130	🟢	🟢	🔵
Renewable Diesel via HTL of Whole Algae/Wood Blend	🔵	🔵	🔵	🔵	⚪	⚪	🟢	🟢	🟢	🟢	🟢	🟠	🟢	🟢	70	130	🟢	🟢	🟠
Renewable Diesel (HEFA)*	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟠	🟠	🟢	🟢	224	224	🟢	🟢	🟠
Farnesane*	🔵	🔵	🔵	🟢	🟢	🔵	🟠	🔵	🔵	🔵	🟢	🟢	🔵	🟠	30	43	🟢	🟢	🔵
Biodiesel (FAME)*	🟢	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🟠	🟠	🟢	🟢	>200		🟢	🟢	🟠

1: Feedstock is 60:40 mix of soybean oil and yellow grease
2: Feedstock is 100% yellow grease
3: Feedstock is 100% soybean oil
4: Future target case
5: GGE/dry US ton

4. Progress and Outcomes

Integrated modeling determined potential impact of co-optimized fuels and engines



Light Duty

RON / MON / S

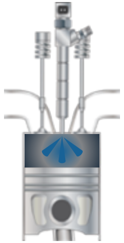
Energy Density

Flash / Boil / Freeze

RVP / HOV

Sooting

Light-Duty and Heavy-Duty Fuels and Combustion Modes



Heavy Duty

Cetane

Energy Density

Flash / Boil / Freeze

Water Sol

Sooting

Refinery Benefits

What is the value of Co-Optima bioblendstocks to the refining industry?

Vehicle Adoption

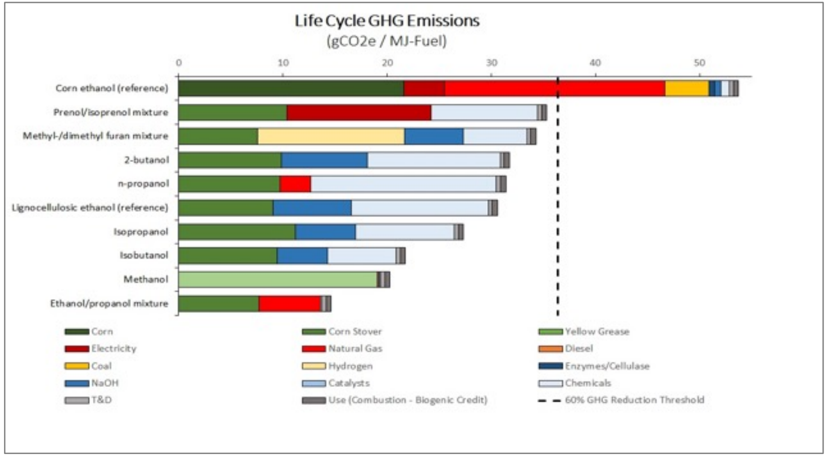
How would Co-Optima fuels and vehicles technology penetrate the market?

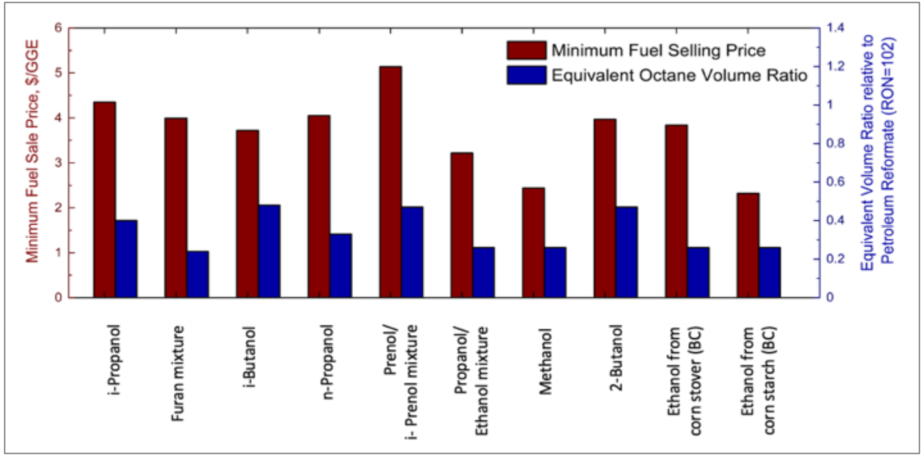
Economy-wide Benefits

Any socio-economic benefits of Co-Optima fuels/vehicle adoption?

4. Progress and Outcomes

Identified top nine MM blendstocks to improve performance, reduce GHG emissions





Blendstocks can achieve >60% GHG emissions reduction relative to petroleum

Top blendstocks exhibit synergistic blending with potential to meet cost targets

Criterion 1: *Enable multimode combustion*

Criterion 2: *Meet advanced biofuel carbon emissions reduction target*

Criterion 3: *Have high market potential*

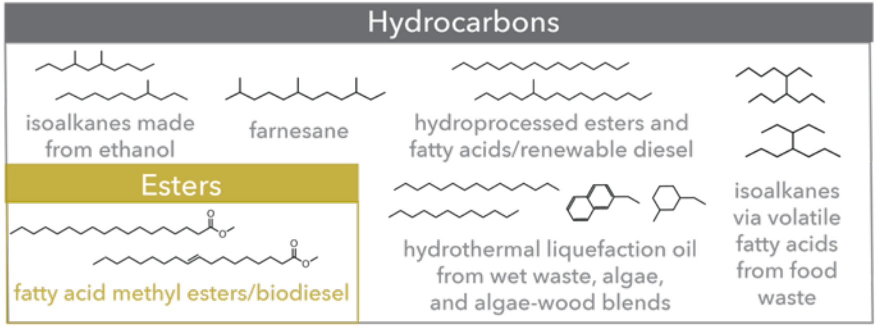
Criterion 4: *Have demonstrated synergistic blending performance for critical fuel properties*

4. Progress and Outcomes

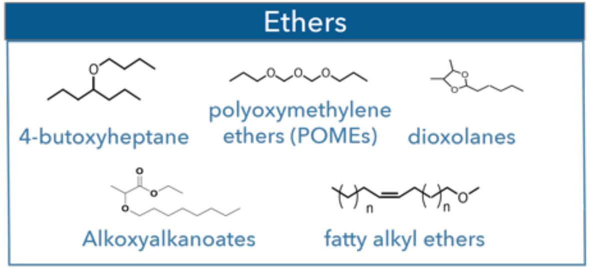
Eleven MCCI blendstocks provide fuel properties and reduce GHG, criteria emissions

- Screened hundreds of mixtures and molecules via fuel property tests (thousands *in silico*), comprising a wide range of hydrocarbon and oxygenate chemistries
- All final candidates offer:
  - CN > 40 (most > 48)
  - LHV > 28 MJ/kg*
  - GHG emissions reduced by 60%+
  - Potential to be produced at $5.50/gge or better
  - Cold weather operability (freezing/cloud point, pour point)
  - Acceptable flash point and other properties
  - Potential to reduce criteria emissions relative to market diesel

MCCI Blendstocks with the Potential to Reduce Emissions and No or Minor Barriers

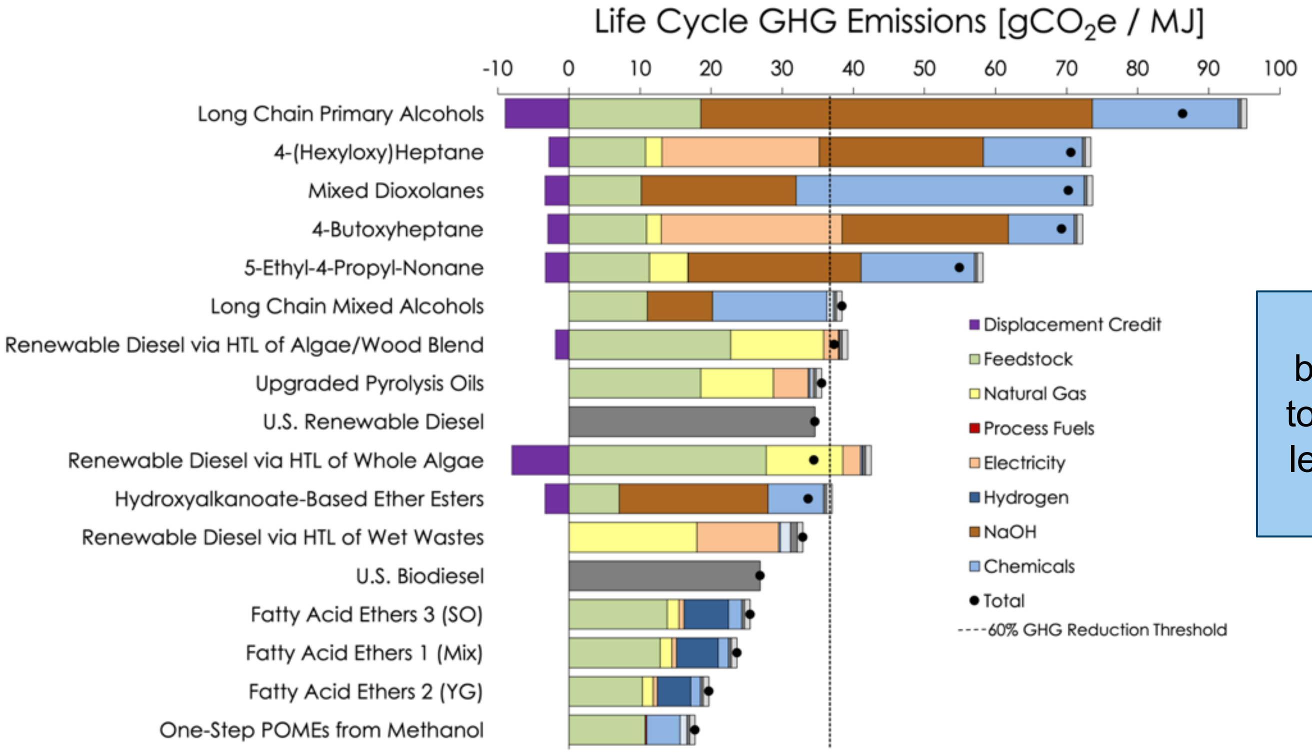


MCCI Blendstocks with Potential to Reduce Emissions With Significant Adoption Barrier(s)



4. Progress and Outcomes

GHG emissions reductions vary; top candidates >60% relative to petroleum emissions



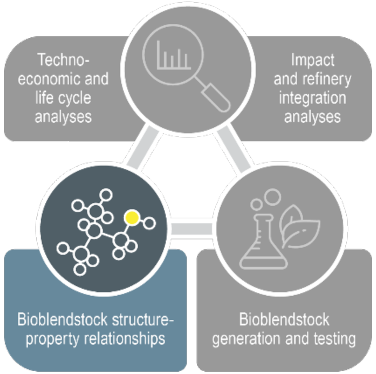
LCA indicates most Top 11 blendstocks have the potential to reduce GHG emissions by at least 60% relative to petroleum diesel

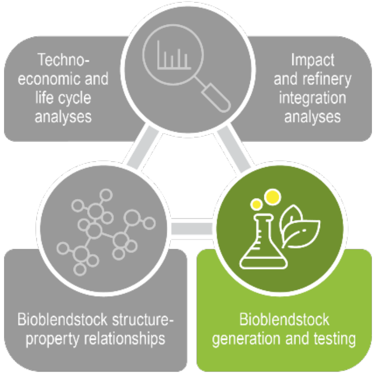
4. Progress and Outcomes

ACI research making progress on defining fuel property targets, SPRs

Goal: Determine target values of fuel properties and ranges for each combustion approach

- Approach – Identify fuel properties which minimize the emissions impact of in-cylinder fuel stratification, while maximizing **phi-sensitivity** and combustion phasing control
- Status
  - High Performance Fuel (HPF) team members helped identify gasoline-range biofuel components with < 98 RON which were not suited for boosted SI but show potential for gasoline-boiling-range HD ACI





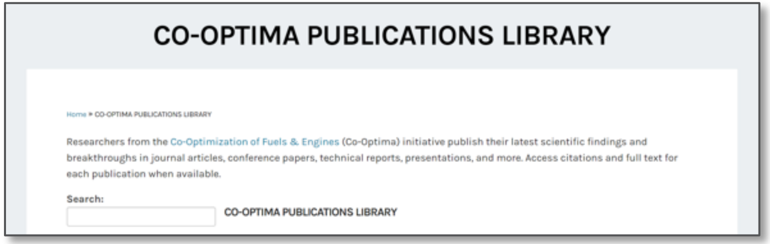
4. Progress and Outcomes

Capstone outputs including key reports and publications advance the SOT

Searchable publication database

(>1300 visits to site in Q1 FY2021)

https://www.energy.gov/eere/bioenergy/co-optima-publications-library-0



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Energy & Environmental Science

Recent capstone reports

- Gaspar et al., “Top Ten Blendstocks for Turbocharged Gasoline Engines”, PNNL-28713
- Farrell et al., “A Transportation Future with Science in the Driver’s Seat”, DOE/EERE-2046
- Dunn et al., “Energy, Economic, and Environmental Benefits Assessment of Co-Optimized Engines and Bio-Blendstocks”, Energy Environ. Sci., 2020, doi: 10.1039/D0EE00716A
- Szybist et al., “What Fuel Properties Enable Higher Thermal Efficiency in Spark-Ignited Engines?”, PECS, 2021, doi: 10.1016/j.pecs.2020.100876
- SAE manuscript. Top 9 manuscripts, in preparation
- Gaspar et al., “Top Eleven Blendstocks Derived from Biomass for MCCI Engines”, under DOE review
- Annual “Year in Review” (YIR) report – among most downloaded on BETO website

4. Progress and Outcomes

Co-Optima technical outcomes have impact with industry and stakeholders

Outcome and Impact

Outcome: Identified performance-advantaged bioblendstocks for LD and HD applications and potential impacts of adoption

Impact: Provide targets to industry with greatest potential for efficiency increase, criteria pollutant emissions reduction and GHG emissions reduction, increasing the bioblendstock value proposition.

Disseminating Results

- ✓ Published 15 papers in Q1 FY2021, 67 (FY20) and 30 (FY21)
- ✓ Conducting upcoming capstone webinars
- ✓ Conducting regular ACS Conference symposium
- ✓ Searchable publication database

Stakeholder Engagement

- ✓ Quarterly EAB meetings
- ✓ Monthly stakeholder calls with >100 participants
- ✓ Conduct meetings with automotive OEMs, biofuel companies, fuel companies, regulators and other stakeholders

Summary of accomplishments

Co-optimizing fuels and engines achieved efficiency, emissions and deployment goals

Light Duty

- Identified blendstocks and engine options to generate 10% fuel economy gain over 2015 baseline

Medium- and Heavy-Duty

- Blendstocks and technology options for potentially lower-cost path to reduced engine-out criteria emissions

Biofuels

- Demonstrated diversification of resource base
- Provided economic options to fuel providers to accommodate changing demands and drivers
- Increased market opportunities for biofuels

Crosscutting Accomplishments

- Provides options to decrease GHG missions by at least 20% for 30% blendstock fraction
- Technology options to stimulate domestic economy and decrease petroleum imports
- Increased clean energy options to add new bio-economy jobs

Summary

Overview	**Developed new fuel and combustion options for more efficient engines with lower harmful emissions, resulting in market pull for the ground transportation sector**
Management	• Multi-discipline, multi-office effort via hypothesis-driven fuel property-based approach • Organized to impact light and heavy duty on-road fleets • Outreach to biofuel and automotive industries, as well as other stakeholders
Approach	• Establish fuel property targets to increase efficiency and and reduce criteria pollutant emissions for each combustion approach • Develop structure-property relationships to identify candidates • Conduct techno-economic and life cycle analyses to refine candidate list • Complete benefits and refinery integration analyses to understand adoption impacts
Impact	• Industry engaged and asking for regular updates • Performance-advantaged candidate bioblendstocks targeted for further development • 123 publications and 5 patents since FY2019, regular ACS symposium, many invited presentations
Progress and Outcomes	• Identified 11 performance-advantaged diesel blendstock candidates reduce GHG emissions • Identified 9 multimode bio-blendstocks with >60% GHG emissions reduction and >10% efficiency gain • Evaluate benefits and impacts of MCCI, MM and KC fuel-engine combinations

Quad Chart Overview

Timeline

Phase 1: Oct 2015 to Sep 2018
Phase 2: Oct 2019 to Sep 2021

	FY2020	Active Project
DOE Funding	*$10,500,000 (BETO)* *$12,000,000 (VTO)*	*$33,250,000 (BETO)* *$33,900,000 (VTO)*

DOE Partner Labs

ANL, INL, LANL, LBNL, LLNL, NREL, ORNL, PNNL, SNL

Barriers Addressed

19ADO-E: Co-development of Fuels and Engine
19At-D: Identifying New Market Opportunities for Bioenergy and Bioproducts

Project Goal

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

End of Project Milestone

Identify at least 5 bioblendstocks that can enable kinetically-controlled combustion while meeting advanced biofuel carbon emissions targets determined by LCA, which have high market potential established by TEA, and have blending performance for fuel properties essential to kinetically-controlled combustion.

Funding Mechanism

Lab Call/Annual Operating Plan

Past Reviewer Comments

1) Better leverage the industry, environmental, and technical expertise of the EAB; review composition of EAB to ensure relevant stakeholder industries and sciences are represented; ensure EAB includes a biochemist and representatives from fuel and vehicle OEMs

Response: In response to this comment, the team has reviewed and updated the membership of the EAB, adding a retired former Cargill research leader and a senior executive from LanzaTech. Over the past year, Co-Optima has had strong and sustained engagement from EAB members, including assistance with outreach.

2) Increase engagement with fuel additive OEMs and other relevant stakeholders; Study fuel impact on lubricants, ignition improvers, etc.

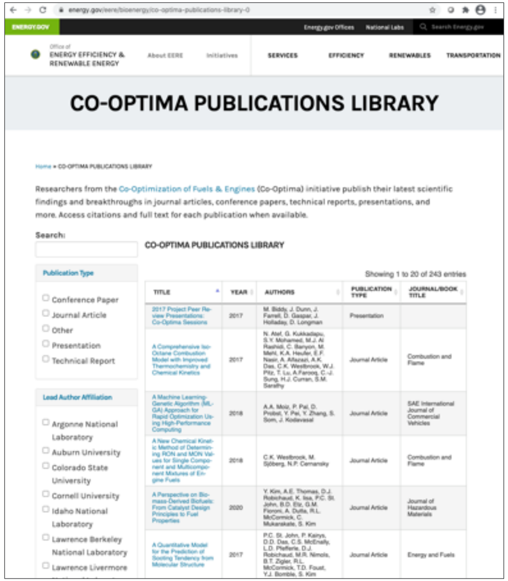
Response: In response to this feedback, Co-Optima initiated fuel-lubricant compatibility research in FY20 (Task A.5.18). Researchers have expanded and continued to engage with companies and consultants in additives market.

3) Make a Co-Optima landing page with all models and data accessible for the public; increase impact by ensuring models are more widely known and utilized; ensure data and results from universities flow to Co-Optima labs

Response: Co-Optima has developed a website (https://cooptima.org) to complement the DOE website (https://www.energy.gov/eere/bioenergy/co-optimization-fuels-engines). The DOE site hosts a searchable Publications Database (https://www.energy.gov/eere/bioenergy/co-optima-publications) and a page with links to Co-Optima developed tools and data (https://www.energy.gov/eere/bioenergy/co-optima-tools-and-data), while the cooptima.org site contains a full listing of Co-Optima capabilities and links to the publication database.

Backup Slides

Publication database and capability pages



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Lead Author Affiliation

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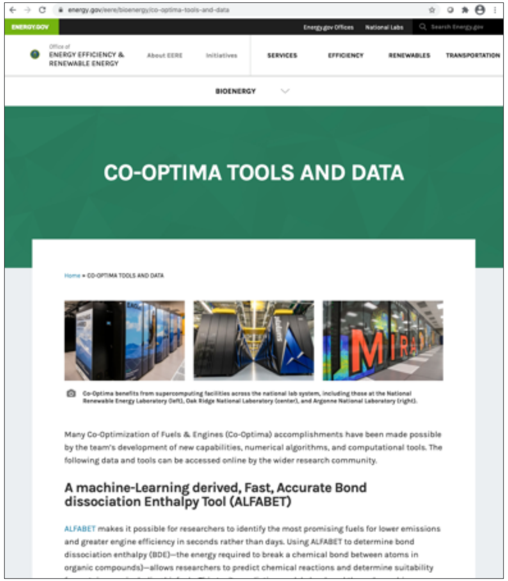
Showing 1 to 20 of 243 entries

TITLE	YEAR	AUTHORS	PUBLICATION TYPE	JOURNAL/BOOK TITLE
2017 Project Peer Review Presentations: Co-Optima Sessions	2017	M. Biddy, J. Dunn, J. Farrell, D. Gaspar, J. Holladay, D. Longman	Presentation	
A Comprehensive Iso-Octane Combustion Model with Improved Thermochemistry and Chemical Kinetics	2017	N. Atef, G. Kukkadapu, S.Y. Mohamed, M.J. Al Rashidi, C. Banyon, M. Mehl, K.A. Heufer, E.F. Nasir, A. Alfazazi, A.K. Das, C.K. Westbrook, W.J. Pitz, T. Lu, A.Farooq, C.-J. Sung, H.J. Curran, S.M. Sarathy	Journal Article	Combustion and Flame
A Machine Learning-Genetic Algorithm (ML-GA) Approach for Rapid Optimization Using High-Performance Computing	2018	A.A. Moiz, P. Pal, D. Probst, Y. Pei, Y. Zhang, S. Som, J. Kodavasal	Journal Article	SAE International Journal of Commercial Vehicles
A New Chemical Kinetic Method of Determining RON and MON Values for Single Component and Multicomponent Mixtures of Engine Fuels	2018	C.K. Westbrook, M. Sjöberg, N.P. Cernansky	Journal Article	Combustion and Flame
A Perspective on Biomass-Derived Biofuels: From Catalyst Design Principles to Fuel Properties	2020	Y. Kim, A.E. Thomas, D.J. Robichaud, K. Iisa, P.C. St. John, B.D. Etz, G.M. Fioroni, A. Dutta, R.L. McCormick, C. Mukarakate, S. Kim	Journal Article	Journal of Hazardous Materials
A Quantitative Model for the Prediction of Sooting Tendency from Molecular Structure	2017	P.C. St. John, P. Kairys, D.D. Das, C.S. McEnally, L.D. Pfefferle, D.J. Robichaud, M.R. Nimlos, B.T. Zigler, R.L. McCormick, T.D. Foust, Y.J. Bomble, S. Kim	Journal Article	Energy and Fuels



energy.gov/eere/bioenergy/co-optima-tools-and-data

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BIOENERGY

CO-OPTIMA TOOLS AND DATA

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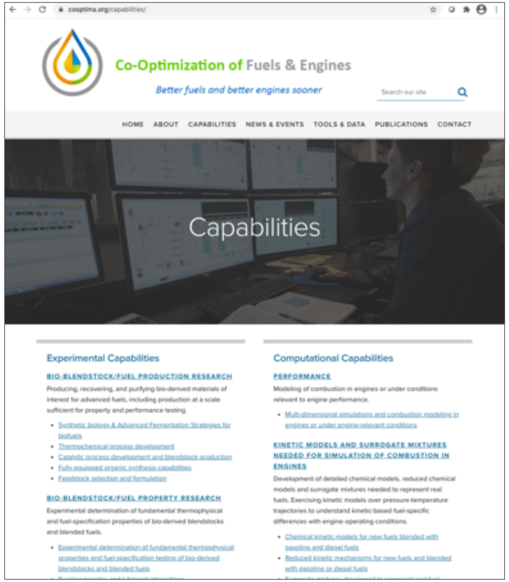
Co-Optima benefits from supercomputing facilities across the national lab system, including those at the National Renewable Energy Laboratory (left), Oak Ridge National Laboratory (center), and Argonne National Laboratory (right).

Many Co-Optimization of Fuels & Engines (Co-Optima) accomplishments have been made possible by the team's development of new capabilities, numerical algorithms, and computational tools. The following data and tools can be accessed online by the wider research community.

A machine-Learning derived, Fast, Accurate Bond dissociation Enthalpy Tool (ALFABET)

ALFABET makes it possible for researchers to identify the most promising fuels for lower emissions and greater engine efficiency in seconds rather than days. Using ALFABET to determine bond dissociation enthalpy (BDE)—the energy required to break a chemical bond between atoms in organic compounds)—allows researchers to predict chemical reactions and determine suitability



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Co-Optimization of Fuels & Engines

Better fuels and better engines sooner

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Capabilities

Experimental Capabilities

BIO-BLENDSTOCK/FUEL PRODUCTION RESEARCH

Producing, recovering, and purifying bio-derived materials of interest for advanced fuels, including production at a scale sufficient for property and performance testing.

- Synthetic biology & Advanced Fermentation Strategies for biofuels
- Thermochemical process development
- Catalytic process development and blendstock production
- Fully equipped organic synthesis capabilities
- Feedstock selection and formulation

BIO-BLENDSTOCK/FUEL PROPERTY RESEARCH

Experimental determination of fundamental thermophysical and fuel-specification properties of bio-derived blendstocks and blended fuels.

- Experimental determination of fundamental thermophysical properties and fuel-specification testing of bio-derived blendstocks and blended fuels

Computational Capabilities

PERFORMANCE

Modeling of combustion in engines or under conditions relevant to engine performance.

- Multi-dimensional simulations and combustion modeling in engines or under engine-relevant conditions

KINETIC MODELS AND SURROGATE MIXTURES NEEDED FOR SIMULATION OF COMBUSTION IN ENGINES

Development of detailed chemical models, reduced chemical models and surrogate mixtures needed to represent real fuels. Exercising kinetic models over pressure-temperature trajectories to understand kinetic-based fuel-specific differences with engine operating conditions.

- Chemical kinetic models for new fuels blended with gasoline and diesel fuels
- Reduced kinetic mechanisms for new fuels and blended with gasoline or diesel fuels

https://www.energy.gov/eere/bioenergy/co-optima-publications

https://www.energy.gov/eere/bioenergy/co-optima-tools-and-data

https://cooptima.org/capabilities

Acronyms

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
CI – Compression ignition
COLT – Co-Optima leadership team
DFI – ducted fuel injection
DFO – directed funding opportunity
DOE – Department of Energy
EAB – external advisory board
EERE – DOE Office of Energy Efficiency and Renewable Energy
EPA – Environmental Protection Agency
FE – fuel economy
FOA – funding opportunity announcement
FP – Fuel Properties team
GGE – gallon of gas equivalent
GHG – greenhouse gas
HoV – heat of vaporization
HD – heavy duty
HPF – High Performance Fuel team
INL – Idaho National Laboratory
ACI – Advanced compression ignition
LANL – Los Alamos National Laboratory
LBNL – Lawrence Berkeley National Laboratory
LC – life cycle
LCA – life cycle 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)
MD – medium duty
MM – multimode combustion
MON – motor octane number
NO_x – nitrogen oxides
NREL – National Renewable Energy Laboratory
OEM – original equipment manufacturer
ORNL – Oak Ridge National Laboratory
PM – particulate matter
PMI – particulate matter index
PNNL – Pacific Northwest National Laboratory
RON – research octane number
S – octane sensitivity (RON – MON)
SI – spark ignition
SPR – structure property relationships
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
WTW – well-to-wheels
XLT – extended leadership team
YIR – year in review
YSI – yield sooting index

Publications & Presentations (1)

330+ publications and presentations, 7 patents

Searchable database available at https://www.energy.gov/eere/bioenergy/co-optima-publications-library-0

FY21 Q1:

- **A Comprehensive Experimental and Improved Kinetic Modeling Study on the Pyrolysis and Oxidation of Propyne** - S. Panigrahy, J. Liang, S.S. Nagaraja, Z. Zuo, G. Kim, S. Dong, G. Kukkadapu, W.J. Pitz, S.S. Vasu, H.J. Curran. Proceedings of the Combustion Institute. 2020. https://doi.org/10.1016/j.proci.2020.06.320
- **A comprehensive experimental and kinetic modeling study of 1- and 2-pentene -** S. Dong, K. Zhang, E.M. Ninnemann, A. Najjar, G. Kukkadapu, J. Baker, F. Arafin, Z. Wang, W.J. Pitz, S.S. Vasu, S.M. Sarathy, P.K. Senecal, H.J. Curran. Combustion and Flame. 2021. https://doi.org/10.1016/j.combustflame.2020.09.012
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- **Discovery of a RON Hyperboosting Phenomenon in Prenol/Gasoline Blends –** A. George. ACS National Fall Conference, Boston, Massachusetts, August 2018.
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- **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 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
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- **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
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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
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- **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
- **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

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- **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
- **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
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- **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
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- **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
- **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.
- **Numerical Prediction of Cyclic Variability in a Spark Ignition Engine Using a Parallel Large Eddy Simulation Approach –** M.M. Ameen, M. Mirzaeian, F. Millo, and S. Som. Journal of Energy Resources Technology, Transactions of the ASME, 140(5):052203, February 2018. doi: 10.1115/1.4039549
- **Octane and Internal Combustion Engine Advancements from a Long(er) Term Perspective: Insights from the Co-Optima Project –** J. Farrell presented at the Fuels 2018 Meeting in Chicago, Illinois, May 22, 2018. https://www.nrel.gov/docs/fy18osti/71673.pdf

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- **On the Interpretation and Correlation of High-Temperature Ignition Delays in Reactors with Varying Thermodynamic Conditions –** M.Y. Tao, A. Laich, P. Lynch, and P. Zhao. International Journal of Chemical Kinetics, 50(6):410-424, June 2018. https://doi.org/10.1002/kin.21170
- **Opportunities for High-Value Bioblendstocks to Enable Advanced Light- and Heavy-Duty Engines: Insights from the Co-Optima Project –** J.T. Farrell. TRB 2018 Annual Meeting, January 2018. https://www.osti.gov/biblio/1418967-opportunities-high-value-bioblendstocks-enable-advanced-light-heavy-duty-engines-insights-from-co-optima-project
- **Optimizing Genetic Manipulation of Microbial Organisms for Production of Multiple Target Chemical Compounds –** L. Whitmore. ACS National Fall Conference, Boston, Massachusetts, August 2018.
- **Parallel Multi-cycle Large-eddy Simulations of an Optical Pent-roof DISI Engine –** N. Van Dam, S. Som, W. Zeng, and M. Sjöberg. ASME ICEF2017, Oct 2017. doi:10.1115/ICEF2017-3603
- **Performance advantaged fuel synthesis and fuel property work –** C. Moore presented at the American Chemical Society Green Chemistry Conference in Portland, Oregon, June 18-20, 2018.
- **Physiochemical Property Characterization of Hydrous and Anhydrous Ethanol Blended Gasoline –** S.A. Shirazi, B. Abdollahipoor, J. Martinson, K.F. Reardon, and B.C. Windom. Industrial and Engineering Chemistry Research, 57(32):11239-11245, August 2018. https://pubs.acs.org/doi/10.1021/acs.iecr.8b01711
- **Polyketide Synthases as a Platform for Chemical Product Design –** A. Zargar, J.F. Barajas, R. Lal, and J.D. Keasling. AIChE Journal 64(12):4201-4207, 2018. https://doi.org/10.1002/aic.16351
- **Prediction of Cyclic Variability and Knock-Limited Spark Advance (KLSA) in Spark-Ignition (SI) Engine --** Z. Yue, D.K. Edwards, S. C. Sluder, and S. Som. Proceedings of the ASME 2018 Internal Combustion Fall Technical Conference, November 2018.
- **Pre-spark Heat Release Effects on Knock-Temperature Relations –** D. Splitter, A. Gilliam, J. Szybist, and J. Ghandhi. AEC MOU Meeting, Argonne National Laboratory, January 29, 2018.
- **Pressure-Temperature Domain Analysis for Insight into Autoignition Events in SI Engines** – J.P. Szybist, and D.A. Splitter. Presented at Oakland University, April 6, 2018.

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- **Probing the Flexibility of an Iterative Modular Polyketide Synthase with Non-Native Substrates in Vitro –** S.C. Curran, A. Hagen, S. Poust, L.J.G. Chan, B.M. Garabedian, T. de Rond, M. Baluyot, J.T. Vu, A.K. Lau, S. Yuzawa, C.J. Petzold, L. Katz, and J.D. Keasling. ACS Chemical Biology, 13(8):2261–2268, 2018. https://pubs.acs.org/doi/10.1021/acschembio.8b00422
- **Production and Upgrading of Fusel Alcohols as High Performance Fuels from Whole Algae Bioconversion** – Monroe et al. ABO Summit – Oral Presentation, October 2017. http://thealgaefoundation.org/upload/Eric_Monroe_ABO_Poster_2017.pdf
- **Production, Blending, and Upgrading of Advanced Renewable Fuels for the Co-Optimazation of Fuels and Engines** – E. Monroe, F. Liu, M. Tran, A. George, J. Gladden, R.W. Davis. Presented as a Poster at ACS 2018, San Francisco, California.
- **Progress in Chemical Kinetic Model Development for Gasoline and Diesel Surrogate Fuels –** S. Wagnon and W. Pitz. Presented to the AEC MOU, Southfield, Michigan, August 15, 2018. https://e-reports-ext.llnl.gov/pdf/362144.pdf
- **Progress Quantifying Fuel Reactivity for Model Validation and Fuel Ranking, across a Range of Combustion Scenarios –** D. Kang and S. Goldsborough. Winter AEC meeting, 2018.
- **Pyrolysis of Cyclopentanone: A Shock Tube and Laser Absorption Study –** E. Ninnemann, A. Laich, S. Neupane, O. Pryor, Z. Loparo, S. Barak, and S. Vasu. 2018 Joint Propulsion Conference, AIAA Propulsion and Energy Forum, AIAA 2018-4474, 2018. 10.2514/6.2018-4474 https://arc.aiaa.org/doi/abs/10.2514/6.2018-4474
- **Reactivity of Novel High-Performance Fuels on Three-Way Catalysts for Control of SI Engine Emissions** – S.S. Majumdar, J. Pihl, and T. Toops. Presentation by J. Pihl at the 2018 CLEERS Workshop, Ann Arbor, Michigan, September 2018. https://cleers.org/wp-content/uploads/formidable/3/2018CLEERS_SreshthaSinhaMajumdar_Web.pdf
- **Reduced Chemical Model for Low and High-Temperature Oxidation of Fuel Blends Relevant to Internal Combustion Engines –** Lapointe, S., K. Zhang, and M.J. McNenly. Proc. Combust. Inst., available online, July 2018. https://doi.org/10.1016/j.proci.2018.06.139
- **Refining Measurement Uncertainties in HCCI/LTGC Engine Experiments --** G. Petitpas, R. Whitesides, J. Dernotte, and J. Dec. SAE Technical Paper 2018-01-1248, 2018. https://doi.org/10.4271/2018-01-1248
- **Replacing Non-Renewable Carbon with Bio-Derived Alternatives –** A.D. Sutton. Presented at Yale University, invited, Chemical and Environmental Engineering Seminar, October 19th, 2018.

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- **Retrosynthetic Analysis of Bio-Derived Fuels, and the Identification of Commodity Feedstocks Critical to Potential Commercialization –** J. Page, P. Koech, D. Malhotra, K. Albrecht, D. Gaspar, L. Whitmore, C. Hudson, A. George, C. Moore, R. Wu, L. Silks, A. Sutton, C. Bailey, A. Zargar, and L. Katz. Presentation and Abstracts of Papers of The American Chemical Society, March 18, 2018.
- **Screening Fuels for Autoignition With Small Volume Experiments and Gaussian Process Classification –** S. Lunderman, G.M. Fioroni, R.L McCormick, M. Nimlos, M.J. Rahimi, and R.W. Grout. Energy Fuels, 2018, 32 (9): 9581–9591. https://pubs.acs.org/doi/10.1021/acs.energyfuels.8b02112
- **Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines –** R. McCormick, G. Fioroni, L. Fouts, and E. Christensen, et al. SAE Technical Papers, Fuels Lubricants, 10(2):442-460, 2017. https://doi.org/10.4271/2017-01-0868
- **Selection Criteria for Sustainable Fuels for High-Efficiency Spark-Ignition Engines with Examination of their Storage Stability, Impact on Engine Knock, and Fine Particle Emissions –** R.L. McCormick. Presented at Colorado State University, May 2018. https://www.nrel.gov/docs/fy18osti/71627.pdf
- **Shock Tube and CO Laser-Absorption Measurements During Cyclopentanone Oxidation –** E. Ninnemann, S. Barak, O. Pryor, W.H. Green, K. Zhang, W.J. Pitz, and S. Vasu. 2018 Spring Technical Meeting of the Eastern States Section of the Combustion Institute, ESSCI 2018.
- **Simultaneously Producing Fuels and Chemicals From Bio-Derived Molecular Building Blocks** – A.D. Sutton. Presented at the 255th American Chemical Society National Meeting, New Orleans, LA, March 18 -22, 2018.
- **Small Ester Combustion Chemistry: Computational Kinetics and Experimental Study of Methyl Acetate and Ethyl Acetate –** A. Ahmed, W.J. Pitz, C. Cavallotti, M. Mehl, N. Lokachari, E. J. K. Nilsson, J.-Y. Wang, A. A. Konnov, S. W. Wagnon, B. Chen, Z. Wang, S. Kim, H.J. Curran, S.J. Klippenstein, W.L. Roberts and S.M. Sarathy. Presented by A. Ahmed at The International Combustion Symposium, Dublin, Ireland, July 2018. https://ccrc.kaust.edu.sa/Pages/Pub-2018-SEC.aspx
- **Sooting Tendencies of Co-Optima Test Gasolines and their Surrogates –** C.S. McEnally, Y. Xuan, P.C. St. John, D.D. Das, A. Jain, S. Kim, T.A. Kwan, L.K. Tan, J. Zhu, and L. D. Pfefferle. Proc. Comb. Inst., available online June 2018. https://doi.org/10.1016/j.proci.2018.05.071
- **Spark Assist for CA50 Control and Improved Robustness in a Premixed LTGC Engine - Effects of Equivalence Ratio and Intake Boost –** G. Gentz, J. Dernotte, C. Ji, and J. Dec. SAE Technical Paper 2018-01-1252, 2018. https://doi.org/10.4271/2018-01-1252
- **Spray–Wall Interactions in a Small-Bore, Multicylinder Engine Operating With Reactivity-Controlled Compression Ignition –** M. Wissink, S.J. Curran, C. Kavuri, and S.L. Kokjohn. Journal of Engine Gas Turbines Power, 140(9), July 30, 2018. doi: 10.1115/1.4039817

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- **Synthesis of a Biofuel Target through Conventional Organic Chemistry –** J.P. Page, J.W. Robinson, K.O. Albrecht, and L. Cosimbescu. Tetrahedron Letters, 59(14):1421-1423, 2018. http://dx.doi.org/10.1016/j.tetlet.2018.02.073
- **Targeting Petroleum Replacements Using Bio-Derived Feedstocks –** C. M. Moore presented at the 22nd American Chemical Society Green Chemistry & Engineering Conference in Portland, Oregon, June 18-20, 2018.
- **Techno-Economic Analysis and Life-Cycle Analysis of Two Light-Duty Bio-Blendstocks: Isobutanol and Aromatic Rich Hydrocarbons –** H. Cai, J. Markham, S. Jones, P. Thathiana Benavides, J.B. Dunn, M. Biddy, L. Tao, P. Lamers, and S. Phillips. ACS Sustainable Chem. Eng., 6(7):8790–8800, 2018.https://pubs.acs.org/doi/10.1021/acssuschemeng.8b01152
- **The Roles of Large-Scale Mixing Structures and Wall Wetting on Ignition and Combustion over a Wide Range of DI SOI in a Dual-Fuel, Heavy-Duty Optical Diesel Engine –** G. Roberts and M. Musculus. AEC Program Review Meeting, Argonne National Laboratory, January 30, 2018
- **The Use of Transient Operation to Evaluate Fuel Effects on Knock Limits Well Beyond RON Conditions in Spark-Ignition Engines –** D. Vuilleumier and M. Sjöberg. SAE paper 2017-01-2234, October 8, 2017. https://doi.org/10.4271/2017-01-2234
- **Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends –** D. Vuilleumier, X. Huan, T. Casey, and M. Sjöberg. *SAE Int. J. Fuels Lubr.* 11(3):247-270, 2018. https://dx.doi.org/10.4271/04-11-03-0014
- **Understanding Chemistry-Specific Fuel Differences at a Constant RON in a Boosted SI Engine –** J.P. Szybist and D.A. Splitter. Fuel, 117:370-381, 2018. https://doi.org/10.1016/j.fuel.2017.12.100
- **Using Ducted Fuel Injection to Attenuate or Prevent Soot Formation in Mixing-Controlled Combustion Strategies for Engine Applications, –** R.K. Gehmlich, C.J. Mueller, D.J. Ruth, C.W. Nilsen, S.A. Skeen, and J. Manin. Applied Energy, 226:1169-1186, 2018. https://doi.org/10.1016/j.apenergy.2018.05.078
- **Using Ducted Fuel Injection to Attenuate or Prevent Soot Formation in a Mixing-Controlled Compression-Ignition Engine –** C.W Nilsen, D.E. Biles, and C.J. Mueller. Advanced Engine Combustion Program-Review Meeting, USCAR, Southfield, Michigan, August 16, 2018.
- **Using Kinetics to Set Expectations for Octane Index for SI and ACI Combustion –** J. Szybist, D. Splitter, S. Wagnon, W. Pitz, and M. Mehl. AEC MOU Meeting, Argonne National Laboratory, January 29, 2018.
- **Vertical LII Diagnostic Development for the Quantification of In-Cylinder Soot Distributions –** Y. Wang, R.K. Gehmlich, M. McNenly, E. Cenker, C.W. Nilsen and C.J. Mueller. Advanced Engine Combustion Program-Review Meeting, Argonne, Illinois, January 31, 2018.

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- **Virtual CFR Engine Knock Model Development and Validation: A Progress Update–** P. Pal et al. AEC Program Review Meeting, Argonne National Laboratory, Illinois, January 29, 2018.

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