2021 DOE Vehicle Technologies Office
Annual Merit Review

Co-Optimization of Fuels and Engines Overview

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Project ID 037

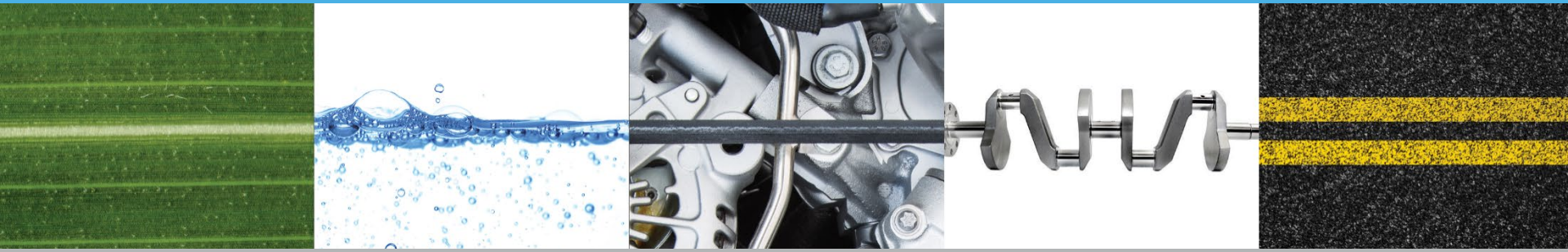
Co-Optima Leadership Team members present and past
Bob McCormick (NREL), Dan Gaspar (PNNL), Anthe George (SNL), John Farrell (NREL), John Holladay (PNNL), Chris Moen (SNL), Paul Bryan (SNL)

And the 200 national laboratory researchers who contributed to Co-Optima

June 24, 2021

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



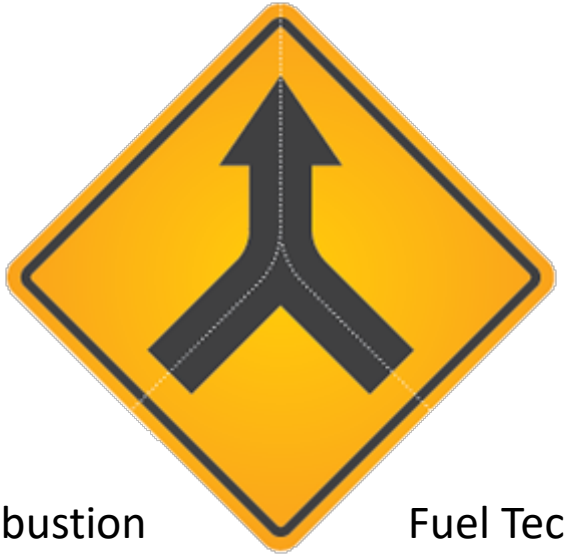
This presentation does not contain any proprietary, confidential, or otherwise restricted information

Special note

This series of presentations is an overview of the 6-year **Co-Optimization of Fuels and Engines** initiative and therefore does not adhere to the standard Annual Merit Review presentation guidance

CO-OPTIMIZATION OF
FUELS & ENGINES

Better fuels. Better engines. Sooner.



Engine / Combustion R&D

Fuel Technologies R&D

Overview

Timeline

- Co-Optima 1.0: FY16-FY18
- Co-Optima 2.0: FY19-FY21

Budget [a]

	VTO ($k)	BETO ($k)	Total ($k)
FY16	11,500	13,700	**25,200**
FY17	12,500	12,000	**24,500**
FY18	8,100	10,000	**18,100**
FY19	10,300	12,000	**22,300**
FY20	12,000	10,500	**22,500**
FY21	10,600	10,400	**21,000**

Barriers [b]

- Lack of robust high-dilution stoichiometric and lean-burn technology and controls
- Inadequate fundamental knowledge base for clean diesel combustion and emissions processes
- Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits
- Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline and diesel fuel

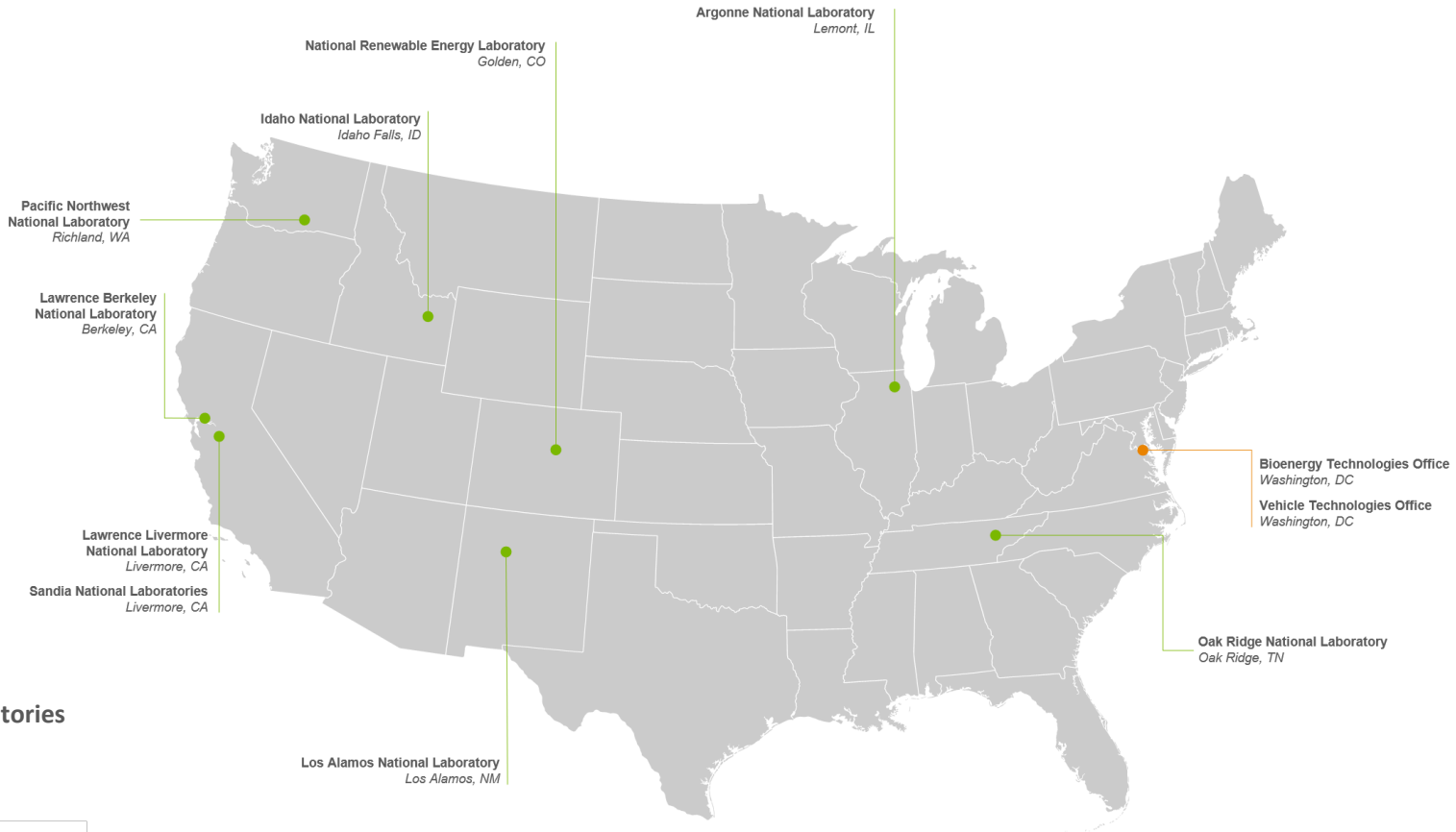
Partners

- Partners include nine national laboratories, 20+ universities, external advisory board, and many stakeholders

a. Task specific budgets will be shown in individual presentations.
b. Barriers 2018 U.S. DRIVE ACEC Tech Team Roadmap.

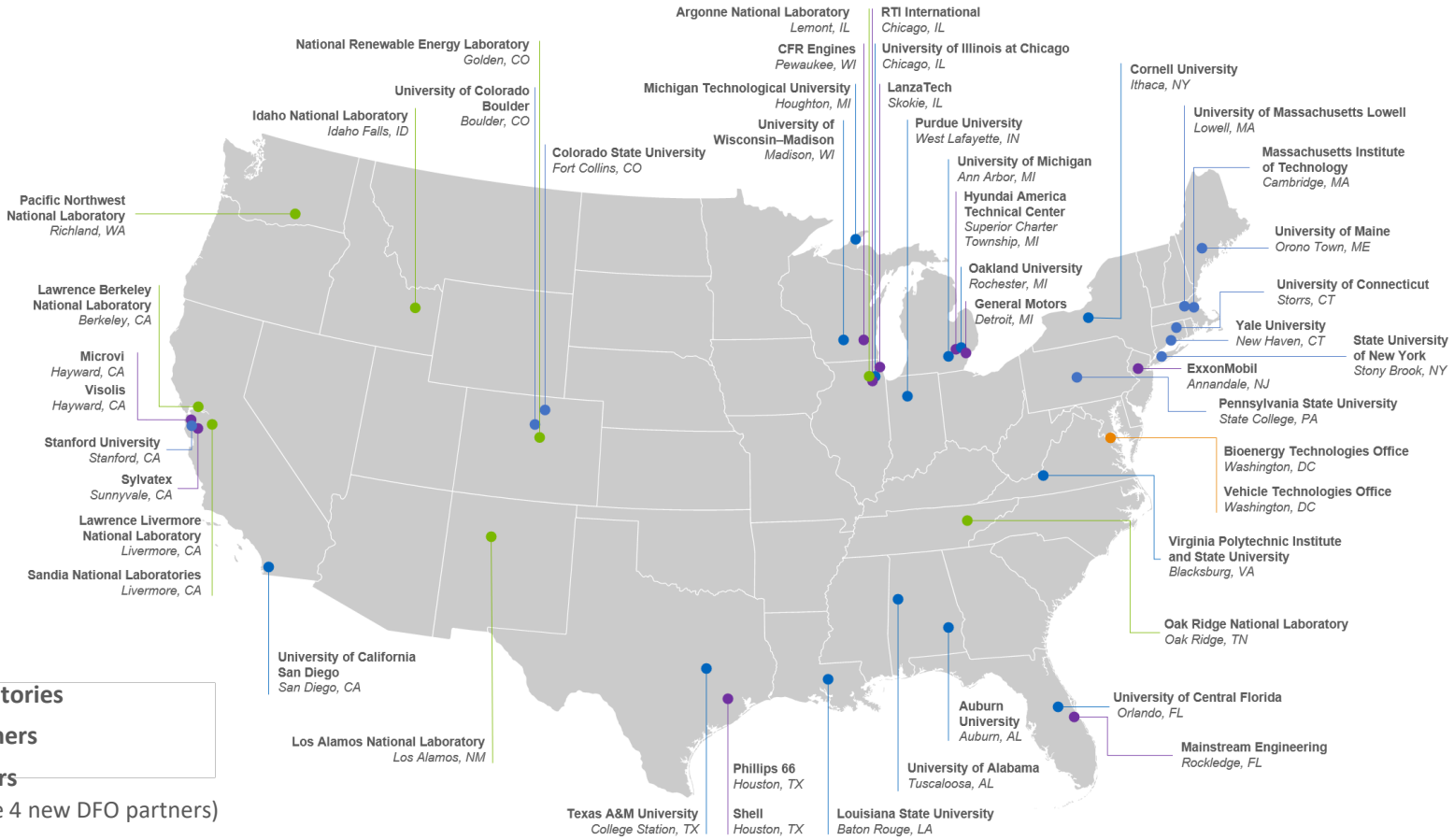
VTO = Vehicle Technologies Office; BETO = Bioenergy Technologies Office

Overview | Initial alignment of national laboratories



- DOE Offices
- National Laboratories

Overview | New partners added through competitive process



- DOE Offices
- National Laboratories
- University Partners
- Industry Partners

(does not include 4 new DFO partners)

Overview | Organizational structure

Board of Directors
(Laboratories 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
(Laboratories and DOE)
Establish vision, define strategy, integrate work plan, oversee execution, evaluate performance, engage stake holders, and team build

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

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

Simulation Toolkit	Advanced Engine Development	Fuel Properties	High Performance Fuels	ASSERT

The team by the numbers

2 DOE EERE offices

100 individual research projects

9 national laboratories

200 national laboratory researchers

17 university-led awards

50 university researchers

8 industry-led awards including DFOs

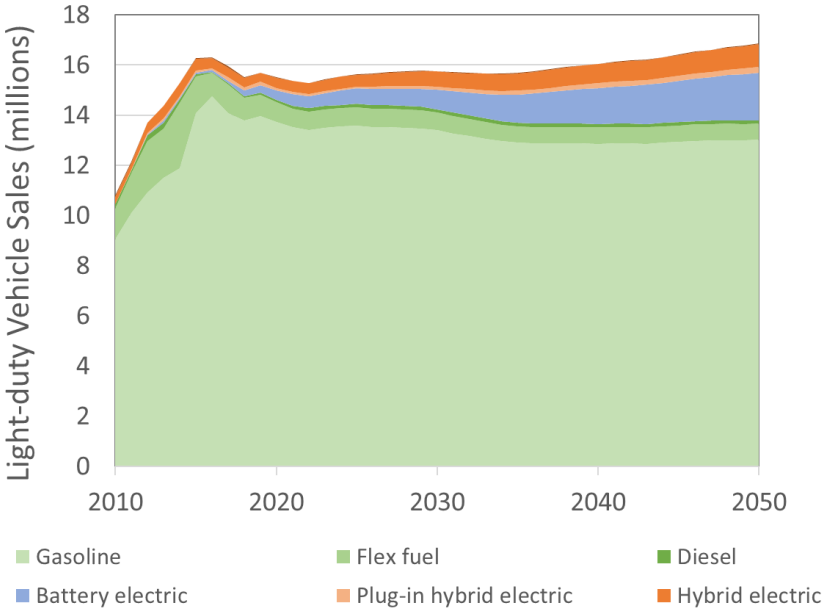
74 stakeholder companies

- **Board of Directors** (semi-annual)
- **External Advisory Board** (quarterly)
- **VTO annual merit review** (annual)
- **BETO peer review** (every other year)
- **DOE leadership updates** (every other week)
- **Stakeholder briefings** (monthly)
- **Co-Optima all-hands** (annual)

Co-Optima drives collaboration across diverse disciplines including biologists, biochemists, chemists, chemical engineers, economists, environmental engineers, mathematicians, mechanical engineers, physicists, …

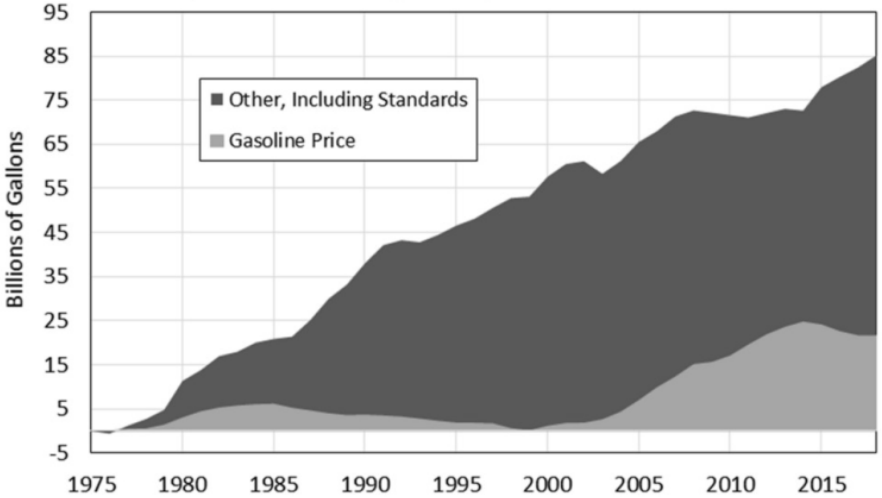
Liquid fuels projected to continue to be important

EIA Annual Energy Outlook projects that internal combustion engines and the use of liquid fuels to dominate transportation for many years



Source: U.S. Energy Information Administration – Annual Energy Outlook 2020

Study estimates fuel economy improvements to US light-duty vehicles from 1975–2018 saved 2T gallons of fuel, 17B tons of CO2



Source: David L. Greene, Charles B. Sims, Matteo Muratori (2020) "Two trillion gallons: Fuel savings from fuel economy improvements to US light-duty vehicles, 1975–2018," Energy Policy, Volume 142, 111517 doi: 10.1016/j.enpol.2020.111517

Relevance | Objectives address VTO program focus areas

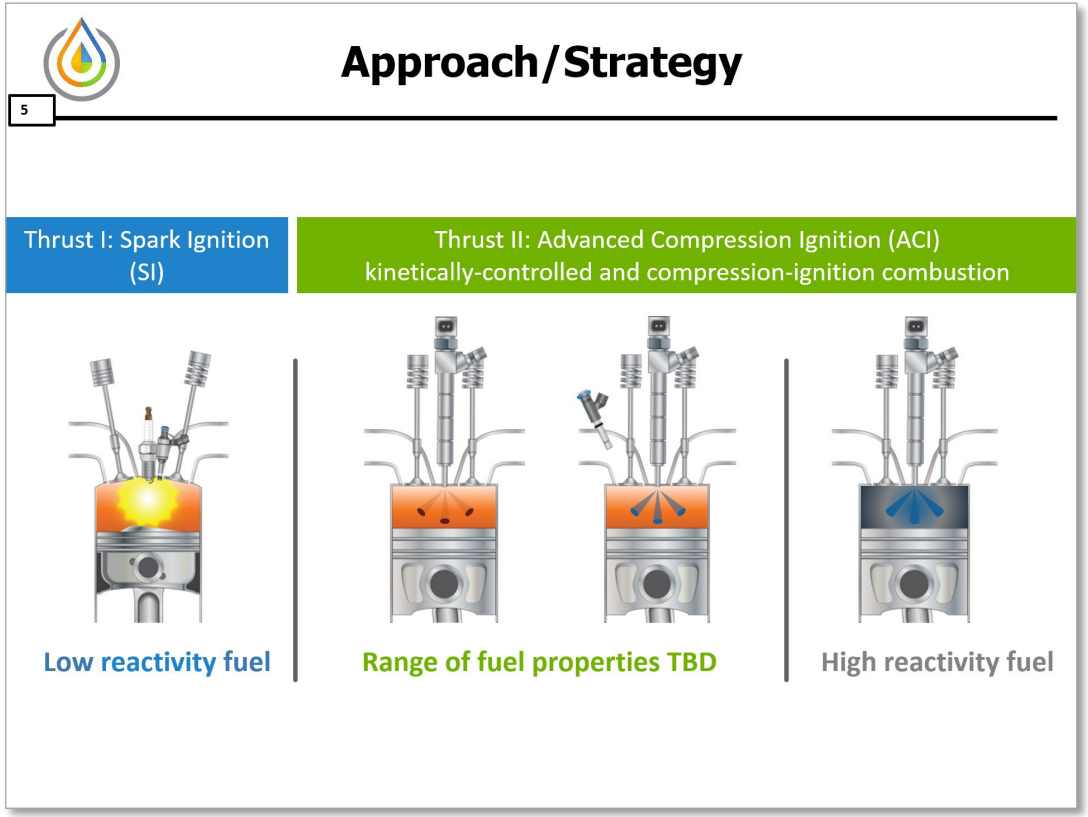
Pre-competitive, early-stage research addresses VTO program* focus to develop better understanding how fuel properties and composition affect advanced combustion systems

- Develop foundational science and knowledge to identify fuel and engine technologies that have the potential to significantly **increase fuel economy and/or reduce emissions**
- Perform comprehensive and consistent blendstock surveys to identify broad range of optionsfor blending with petroleum base stocks to achieve key target properties; broad range of options important to **energy security**
- Develop and make use of validated new models and analyses to accelerate knowledge discovery and experiments
- Demonstrate blendstock candidates that can be produced from renewable domestic biomass feedstocks that have the potential to be **affordable, scalable, sustainable, and compatible**

* https://www.energy.gov/eere/vehicles/advanced-combustion-systems-and-fuels

Approach | In the beginning …

- **Co-Optima was originally called Optima and originated from a multi-laboratory DOE "Big Idea"**
- **Research thrusts focused on spark-ignition and compression-ignition combustion and fuels**
- **Focus was reworked based on industry recommendations**



Source: VTO AMR, June 9, 2016

Approach | Structure reworked to align with LD and MD/HD

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

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

Light-Duty

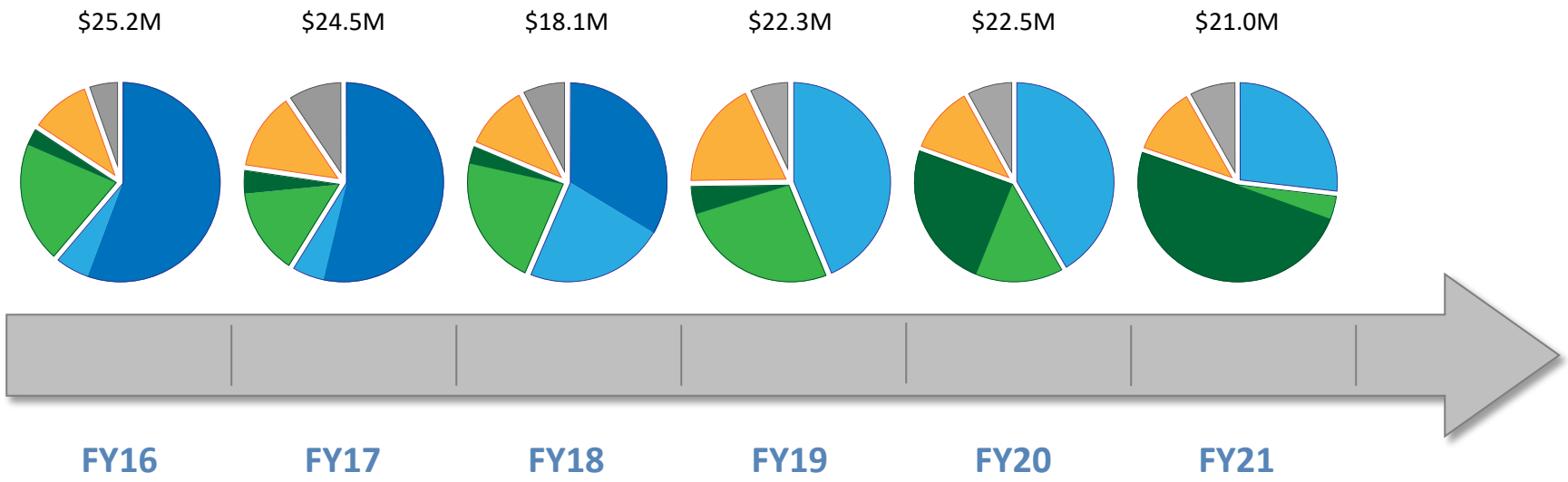
2030 Goal | 10% fuel economy improvement beyond expected 25% increase from base engine improvements

Medium/Heavy-Duty

2030 Goal | 4% fuel economy improvement and lower cost path to meeting criteria emissions regulations

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

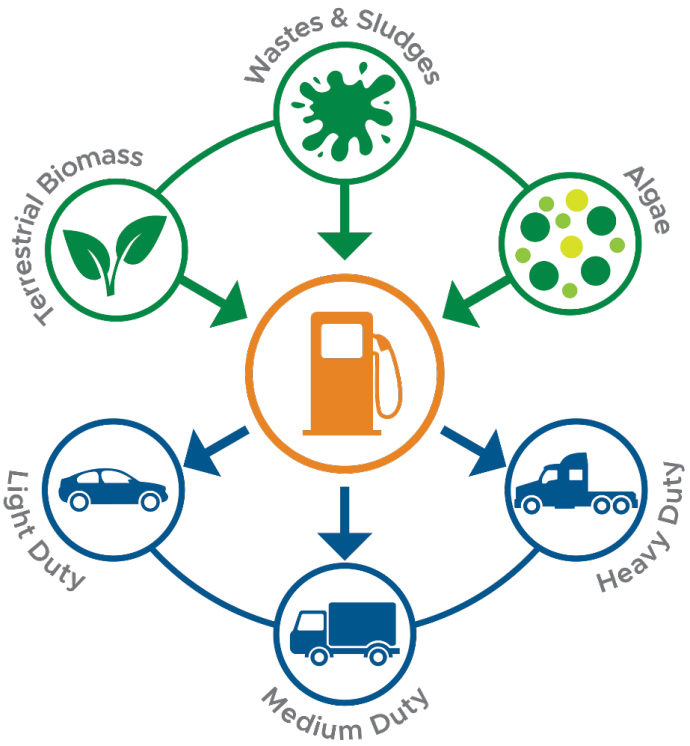
Approach | Planned shift in focus over the course of the initiative



LD Boosted SI | LD Multimode SI/ACI | MD/HD MCCI | MD/HD ACI | Crosscutting | Project Management

Approach | Initiative scope

- **Focus only on liquid fuels**
- **Identify blendstocks to blend into petroleum base fuel (up to 30% by volume)**
- **Identify fuel properties that optimize engine performance, independent of composition**
- **Considering only non-food-based biofuel feedstocks**
- **Assessing WTW emissions (GHG, water, etc)**
- **Considering hybridized/non-hybridized powertrain solutions**
- **Provide data, tools, and knowledge to stakeholders**

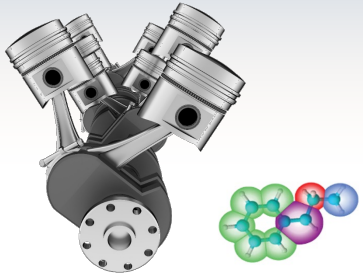


Approach | Well integrated with BETO

- **Important to emphasize that Co-Optima is a joint program across VTO and BETO**
- **BETO specific goals**
  - Identify fuel blendstocks with significantly lower well-to-wheel CO2 emissions
  - Diversify resource base
  - Provide economic options to accommodate changing global fuel demand
  - Increase supply of domestically sourced biofuels by up to 25 billion gallons a year
- **For a more complete understanding of the BETO scope and accomplishments, please see the recent presentations from the BETO peer review**
  - https://www.energy.gov/eere/bioenergy/2021-project-peer-review

Approach | Addresses three critical questions with two hypotheses

What fuels do engines really want?



What fuel options work best?

What will work in the real world?

Central Engine Hypothesis

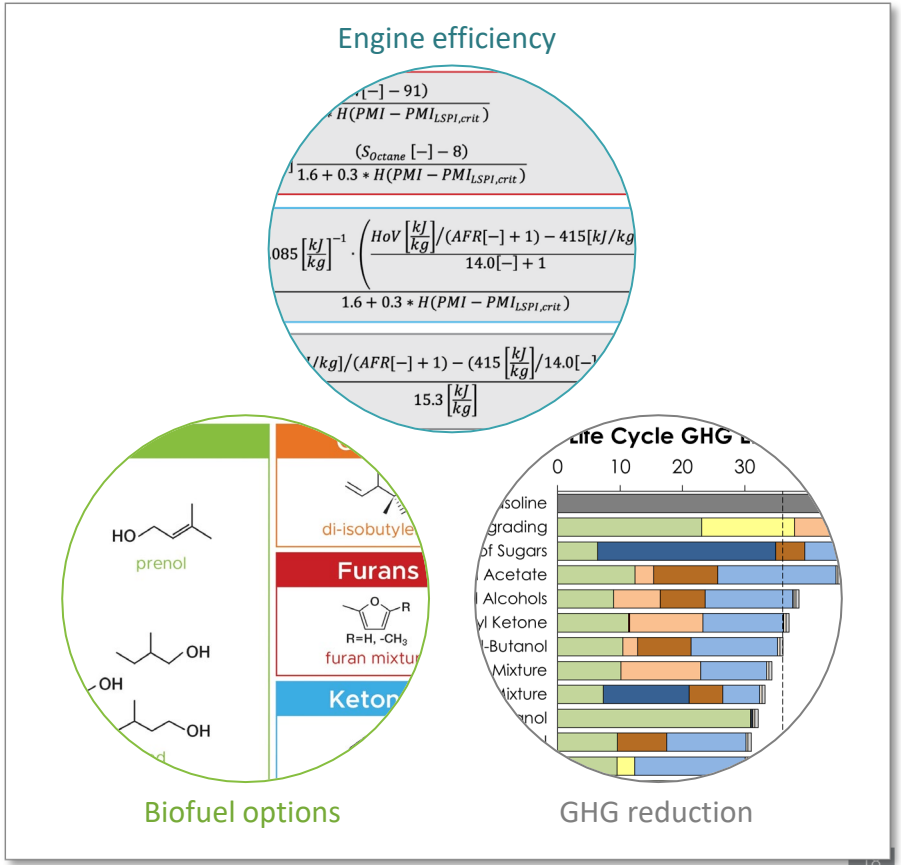
There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range.

Central Fuel Hypothesis

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

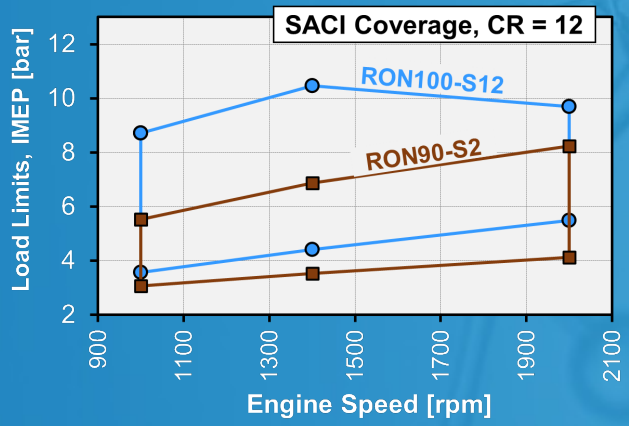
Notable Accomplishments | LD Spark-ignition gasoline-range

- **Identified fuel properties with highest impact on efficiency:**
  - Research octane number (RON)
  - Octane sensitivity (S)
  - Heat of vaporization (HoV)
- **Identified blendstocks with highest potential for improvement:**
  - Alcohols
  - Iso-olefins
  - Alkylfurans
- **Characterized potential reduction in life cycle greenhouse gas emissions for blendstocks with highest potential**



Notable accomplishments | LD SI Multimode gasoline-range

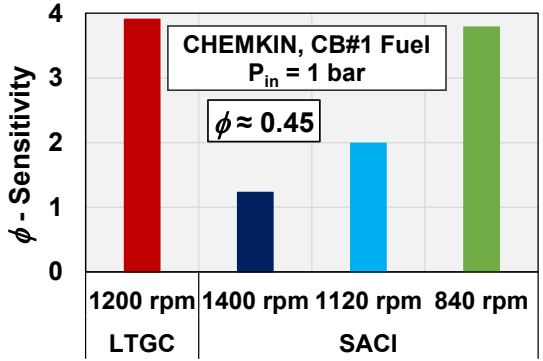
- **Octane requirements of Multimode engines that use SACI is aligned with Boosted SI**
- **High RON, high-S gasolines provide greater load coverage with lean and efficient SACI**



S – Octane Sensitivity
SACI – Spark Assisted Compression Ignition

Enhanced phi-sensitivity typically does not provide benefits for LD SACI

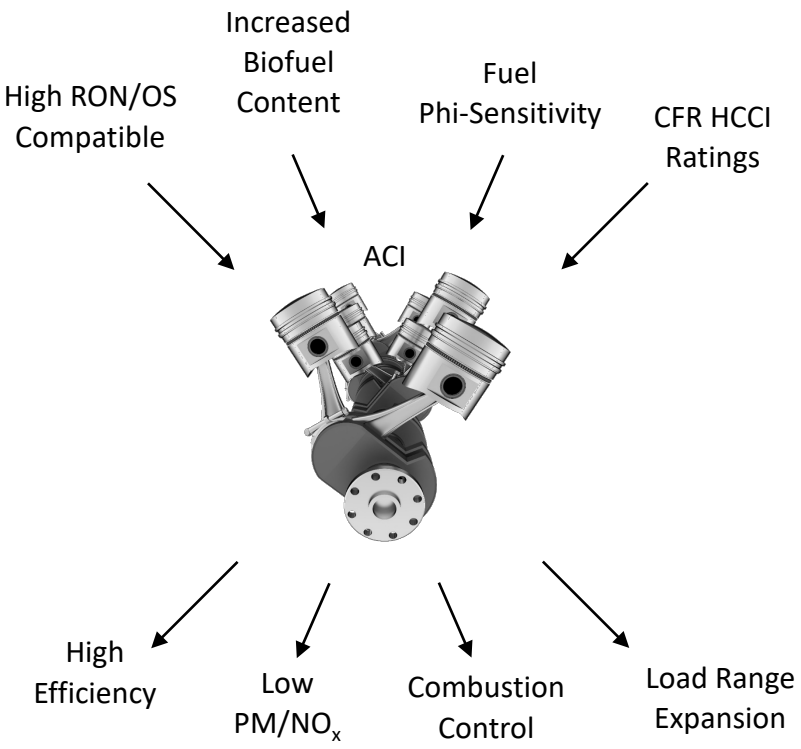
Flame-induced compression is fast and leaves less time for the ITHR that is critical for fuel phi-sensitivity



ITHR – Intermediate Temperature Heat Release
CB#1 – Custom Blend with 12.4% isobutanol
LTGC – Low Temperature Gasoline Combustion (MD/HD ACI)

Notable accomplishments | ACI

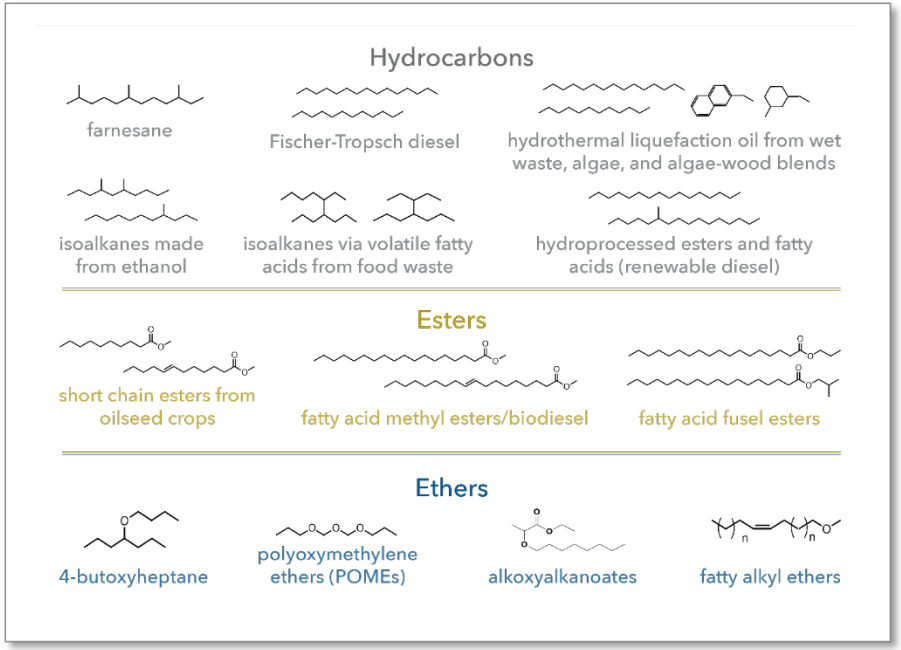
- **High RON, high octane sensitivity gasolines (suitable for boosted SI/MM engines) can be compatible with MD/HD ACI engines**
- **ACI combustion demonstrated diesel-like or higher efficiency with substantial reductions in PM/NO_x**
- **Lean HCCI fuel ratings significantly improved ACI reactivity prediction accuracy over RON/MON/OI**
- **Chemical kinetics-based fuel design demonstrated:**
  - Improved fuel phi-sensitivity
  - Higher RON and octane sensitivity (also benefiting SI engines)
  - Increased biofuel content



ACI – Advanced Compression Ignition; HCCI – Homogeneous Charge Compression Ignition

Notable Accomplishments | MD/HD diesel-range

- **Thirteen blendstocks identified with potential to reduce GHG by 60%+ and criteria emissions**
- **Improved understanding of the potential of bioblendstocks to reduce soot enabling higher levels of dilution to lower NOx**
- **New insights into synergies of ducted fuel injection (DFI) and bioblendstocks to for 100x reduction in soot (10x from DFI, 10x from bioblendstocks)**



Accomplishments | Significant details to be presented later today…

10:00 AM	FT037	Co-Optimization of Fuels and Engines (Co-Optima) (Robert Wagner, ORNL)
10:30 AM	FT090	Bioblendstock Generation and Analysis (Anthe George, SNL)
11:00 AM	FT094	Fuel Properties and Kinetics (Gina Fioroni, NREL)
11:30 AM	FT091	Fuel Effects in Boosted, Spark-Ignition Combustion (Jim Szybist, ORNL)
12:00 PM	FT092	Fuel Effects on Multimode Engine Operation (Magnus Sjoberg, SNL)
1:40 PM	FT093	Diesel-like Fuels, Combustion, and Emissions (Steve Busch, SNL)
2:10 PM	FT096	Advanced Compression Ignition Combustion Engines: Gasoline-Range Fuels (Christopher P. Kolodziej, ANL)
2:40 PM	FT097	Summary and Future Directions (Bob McCormick, NREL)

Accomplishments | Summarized in year-in-review documents

- **This is the best resource for a high-level overview of accomplishments**
- **FY16 – FY20 now available online**

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

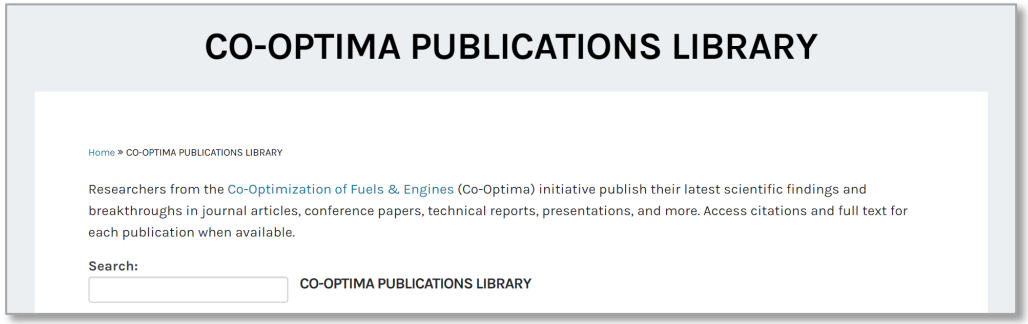
Accomplishments | Capstone reports and publications available for download

Recent capstone reports

- Gaspar et al., "Top Ten Blendstocks for Turbocharged Gasoline Engines", **PNNL-28713** (download)
- Farrell et al., "A Transportation Future with Science in the Driver's Seat", **DOE/EERE-2046** (download)
- Dunn et al., "Energy, Economic, and Environmental Benefits Assessment of Co-Optimized Engines and Bio-Blendstocks", **Energy Environ. Sci.**, 2020, DOI: 10.1039/D0EE00716A (download)
- Szybist et al., "What Fuel Properties Enable Higher Thermal Efficiency in Spark-Ignited Engines?", **Progress in Energy and Combustion Science** (download)

Searchable publication database (more than 1000 visits to site)

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



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

Energy & Environmental Science

Accomplishments | Additional Capstone reports planned

Area	Topic
LD Multimode ACI	Blendstocks and Benefits: MM Dashboard Report and Subsequent Analyses
	What is the potential for fuel economy enhancement via co-optimized MM fuels and engines
MD/HD	MCCI Top 14
	MCCI Combustion Opportunities
	MD/HD Benefits Analysis/Comprehensive Analysis Report
Crosscutting	Integrated modeling approaches and applications to co-optimization
	From E10 to C30 to NZC liquid transportation fuels – how might we make this transition?
Future	What do we now know about combustion and what should come next?

Accomplishments | Capstone webinar series is underway …

MAR 25

How can co-optimized fuels and spark-ignition engines enhance efficiency while reducing carbon emissions of light-duty passenger vehicles?

Daniel Gaspar
Pacific Northwest National Laboratory

Jim Szybist
Oak Ridge National Laboratory

APR 29

How can fuels and combustion reduce pollutants from future diesel engines?

Bob McCormick
National Renewable Energy Laboratory

Charles Mueller
Sandia National Laboratories

MAY 27

What environmental and economic benefits might be realized by co-optimizing fuels and spark-ignition engines for light-duty passenger vehicles?

Troy Hawkins
Argonne National Laboratory

JUN 24

What environmental and economic benefits might be realized by co-optimizing fuels and engines for medium-duty and heavy-duty commercial vehicles?

Avantika Singh
National Renewable Energy Laboratory

AUG 26

What unconventional engine-fuel combinations show the greatest promise for efficiency improvements beyond current LD/MD/HD technologies?

Magnus Sjöberg
Sandia National Laboratories

SEP 30

Co-optimization of fuels and engines: past, present, and future—what did we learn and where do we go next?

Robert Wagner
Oak Ridge National Laboratory

Daniel Gaspar
Pacific Northwest National Laboratory

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

Collaboration | Multiple laboratories, universities, etc.

- **DOE cross-office collaboration** to bridge expertise and resources of VTO and BETO
- **Cross-laboratory collaborations** to bridge unique expertise, facilities, and modeling expertise
- **Laboratory-university collaborations** to address gaps in resources
- **Laboratory-industry interactions** including the donation of engine hardware
- Close interactions with analogous program **"Fuel Science Center"** Cluster of Excellence at RWTH Aachen University
- Significant **industry input** through company visits, monthly webinars, every-other-month report outs at the DOE-industry Advanced Engine Crosscut meeting, and through an **External Advisory Board**

Collaboration | Annual all-hands meeting brings us all together

This annual event has been the single most important forum for improving trust and driving collaboration across the national laboratories

Summary

Relevance

- Addresses VTO program focus to develop better understanding how fuel properties and composition affect advanced combustion systems
- Supports identification of cleaner technology pathways to reduce energy costs and increase energy security through diversification

Approach

- Integrate unique expertise and facilities of national laboratories, universities, and industry in experimentation, modeling, and analyses

Technical Accomplishments

- Delivering foundational science to develop fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals for LD, MD, and HD sectors
- Documented in AMR presentations, recent BETO peer review presentations, and FY20 year-in-review document

Collaborations

- Initiative-level collaborations across nine national laboratories, 20+ universities, two DOE offices, industry, and other stakeholders

Proposed Future Research

- This is the end of the current phase of the Co-Optima initiative

Any proposed future work is subject to change based on funding level