2021 DOE Vehicle Technologies Office

Annual Merit Review

Summary and Future Directions

Principal Investigator: Robert L. McCormick
Organization: National Renewable Energy Laboratory

Co-Optima Leadership Team Members Present and Past:
Robert Wagner (ORNL), Dan Gaspar (PNNL), Anthe George (SNL), John Farrell (NREL), John Holladay (PNNL), Chris Moen (SNL), Paul Bryan (SNL)

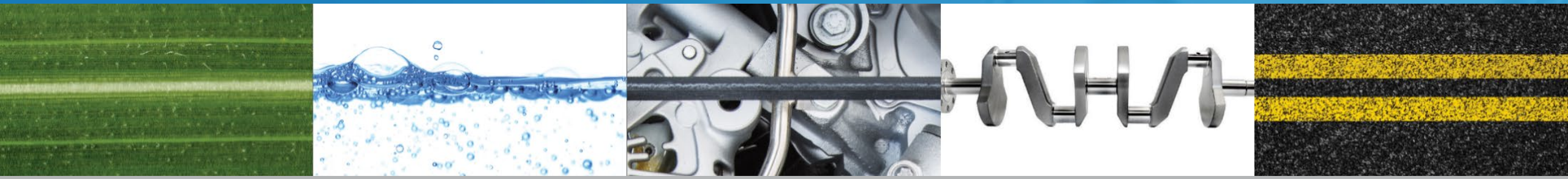
And the 200 national laboratory researchers who contributed to Co-Optima

Project ID # 097

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

Outline

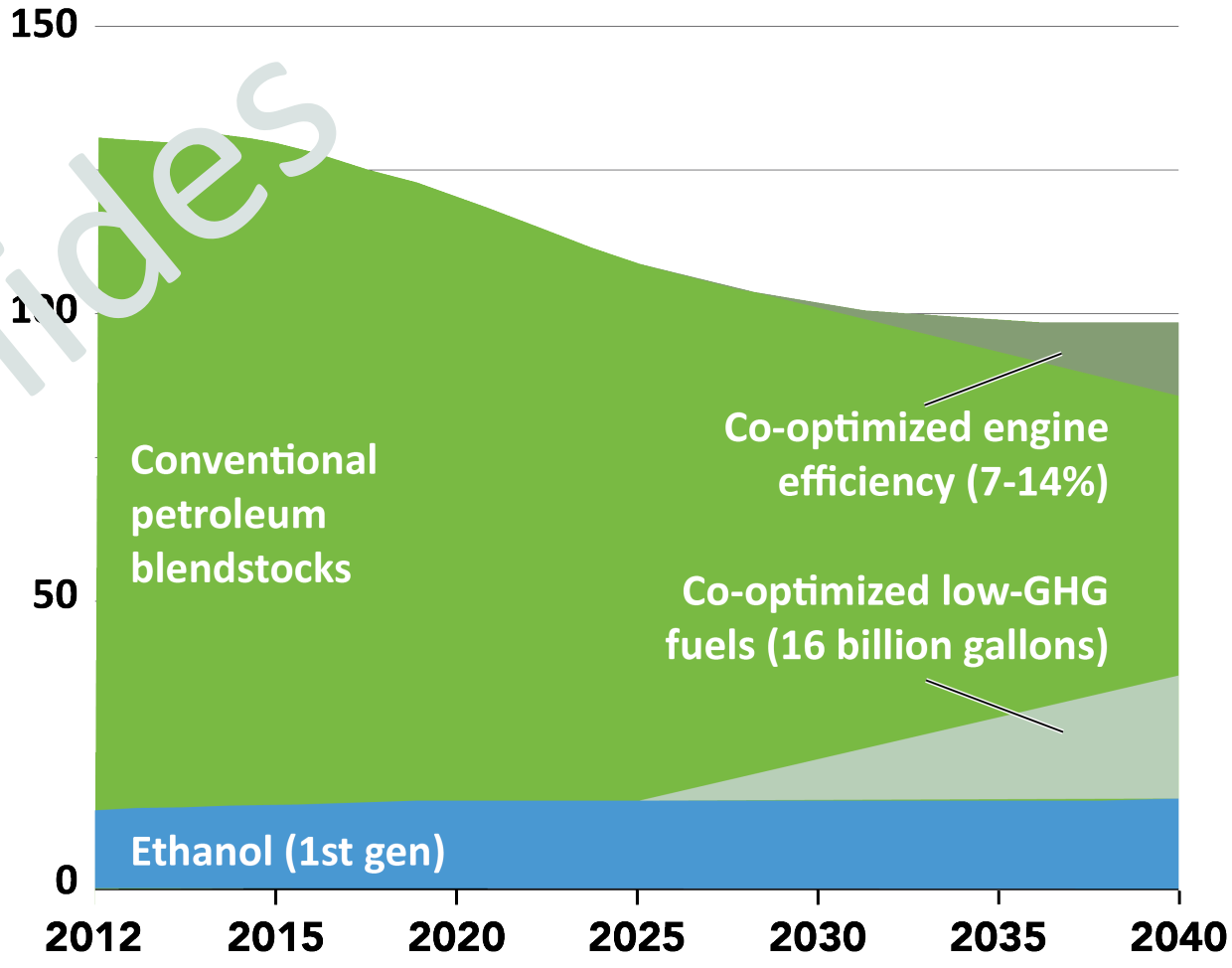
- What Co-Optima was like in 2016
- Summary of timeline and goals
- Major outcomes
- Ongoing work FY21 and FY22 wrap up
- How the world has changed
- The case for low-carbon liquid fuels
- Future work recommendations

Remember 2016?

30% per vehicle petroleum reduction via efficiency and displacement

2016 Slides

Light duty fuel consumption (billion gallons/year)



source: EIA 2014 reference case

National goal:

80%

reduction in transportation GHG by

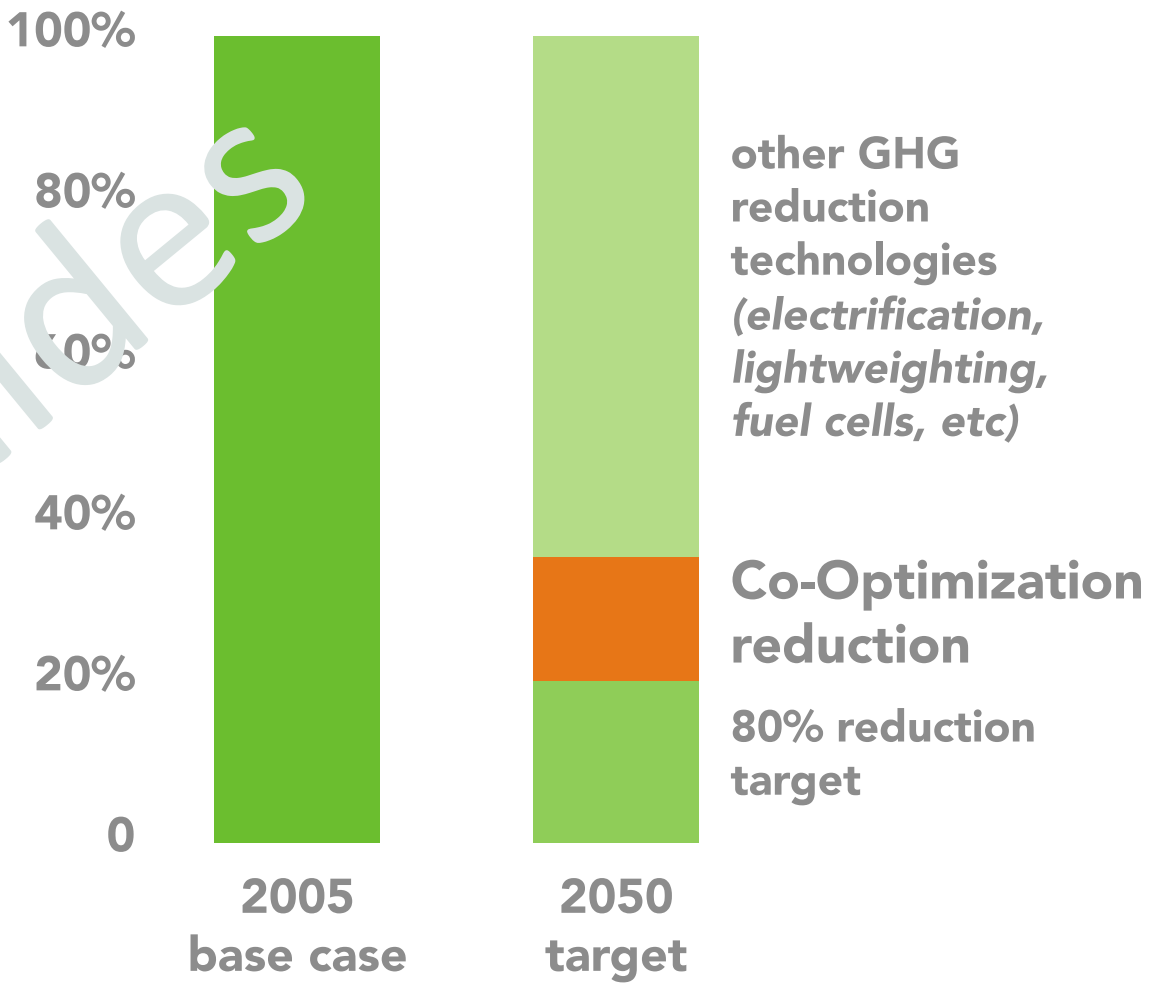
2050

Co-Optimization:

9-14%

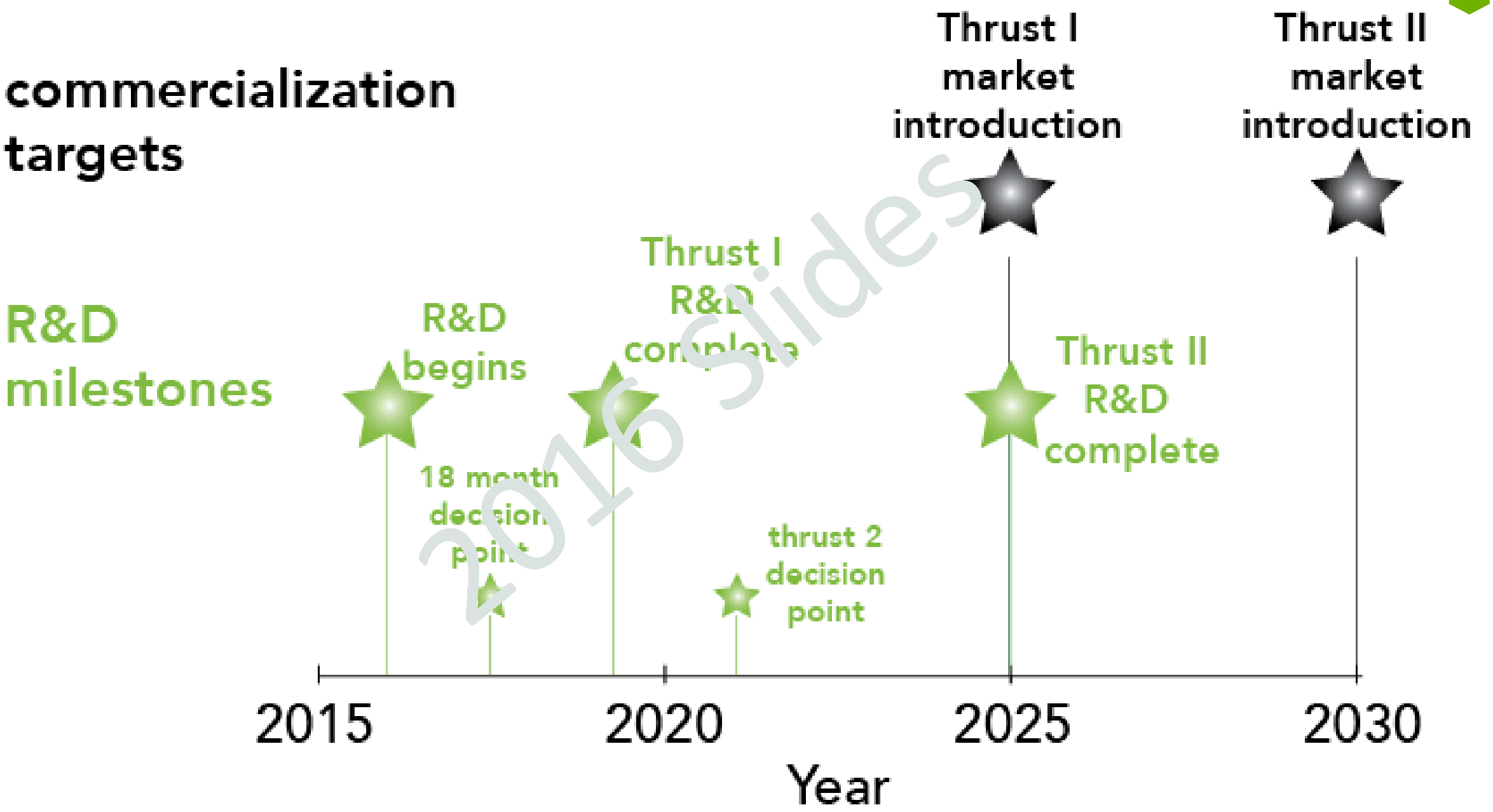
GHG reduction

(beyond "business as usual")



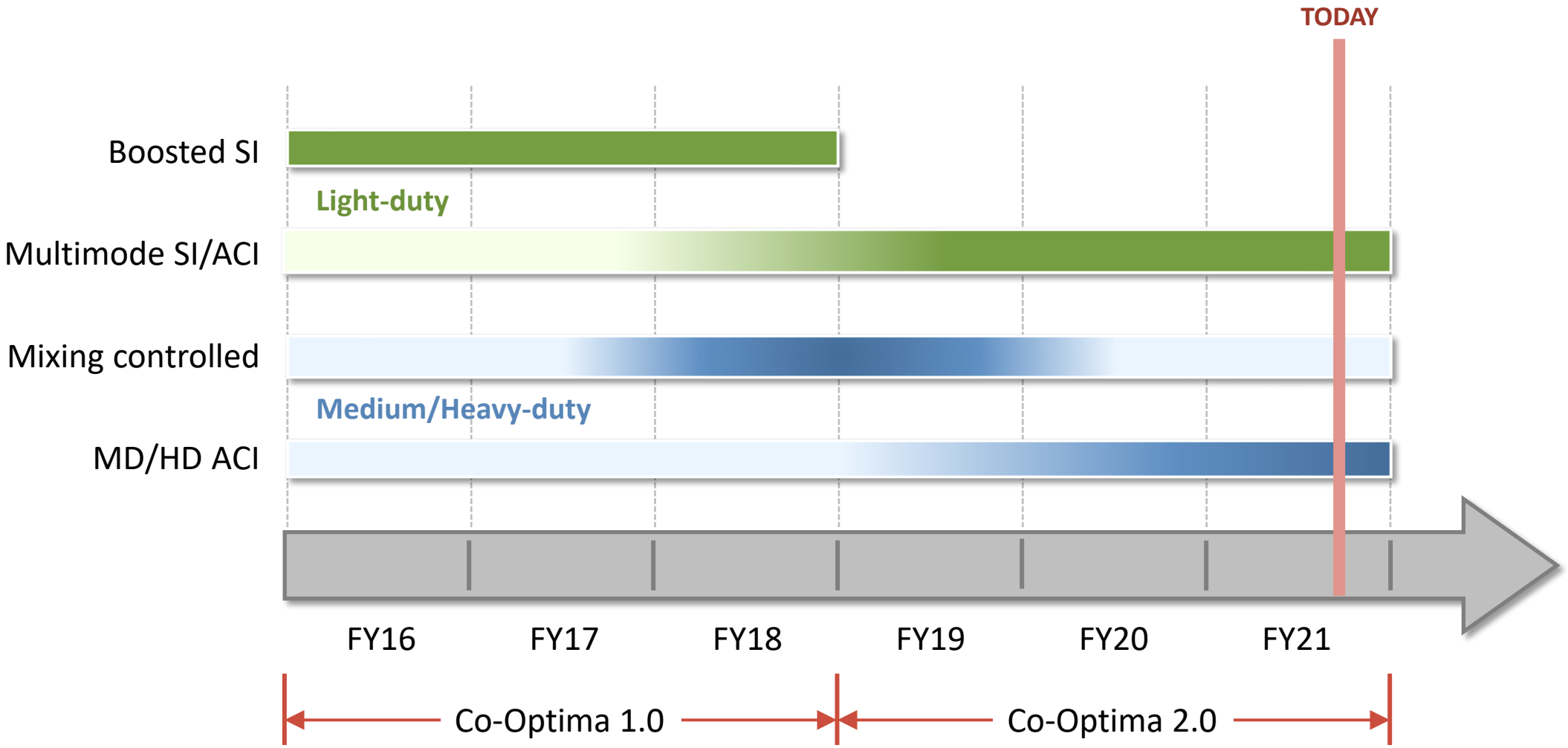
2016 Slides

commercialization targets



2016 slides

Timeline


TODAY
Boosted SI
Light-duty
Multimode SI/ACI
Mixing controlled
Medium/Heavy-duty
MD/HD ACI
FY16
FY17
FY18
FY19
FY20
FY21
Co-Optima 1.0
Co-Optima 2.0

Co-Optima goals aimed to increase sustainability of transportation

Provide technology options for fuels and engines

Biofuels

- Increase market opportunities for biofuels
- Diversify resource base
- Provide economic options

Engines

- Increase fuel economy
- Reduce total cost of ownership
- Reduce emissions

Light Duty

- 10% fuel economy gain over 2015 baseline
- Provide market pull for use of low CI blendstocks

Medium- and Heavy-Duty

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

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

Outcomes Addressing Goals

- Identified and developed fuels from woody biomass, algae, and waste
  - With fit-for-purpose and high-performance properties for SI and MCCI engines
  - Modeled costs below $5.50/gge
  - Reduced blendstock life-cycle carbon intensity (g CO2-eq/MJ fuel) by 60% or in many cases significantly higher (20% reduction for 30% blends)
- Demonstrated blendstocks that enable a 10% efficiency improvement for boosted SI engines
  - A further 6 to 12% efficiency gain possible with MM engines – being confirmed in ongoing work
- Proof of concept that ducted fuel injection, combined with oxygenate blending, can reduce diesel in-cylinder soot by a factor of 100, with large NOx reductions from exhaust gas recirculation
- Research on gasoline compression ignition is showing a 4% increase in efficiency relative to conventional diesel at low load – research is ongoing in FY21

Cross-cutting Outcomes

- New approaches to fuel property measurement using small volumes
- Molecular structure – fuel property relationships and machine learning models for property prediction
- Dramatic improvement in scope and fidelity of combustion kinetic simulations
- CFD simulations for high fidelity prediction of the behavior of evaporating fuel sprays and other complex engine phenomenon
- Integration of simulations across scales from molecular (chemical kinetics) to vehicle drive cycle emissions
- Over 280 publications with many more in preparation

Demonstrated capabilities as a collaboration

- **Cross-office collaboration (VTO – BETO)**
- **Approximately 130 individual projects, over 200 researchers**
- **Biologists, biochemists, chemists, chemical engineers, economists, environmental engineers, mathematicians, mechanical engineers, physicists, …**
- **Project management with two DOE offices and all nine national laboratories**
  - Leadership team (four national laboratories)
  - Five technical teams (lead and deputy for each team)
  - Steering committee (all nine national laboratories)
  - Full-time project manager

- **External advisory board made up of industry and university leaders**
- **Primed to collaborate on future challenges**

MCCI and ACI Research FY21 to FY22

Multimode (FY21)

- Complete TEA/LCA and refinery benefits, prepare manuscripts on MM blendstocks
- Develop a fuel property metric to capture fuel autoignition behavior under ACI conditions relevant to SI/ACI multimode engines
- Modeling to understand MM fuel economy gain potential using pervious experimental work

MCCI (FY21, FY22 wrap up)

- TEA/LCA, structure property relationships, ecotoxicity, and kinetics research
- Fuel property impacts on catalyst heating operation and emission control catalysts
- Finalized blendstock and refinery integration analysis

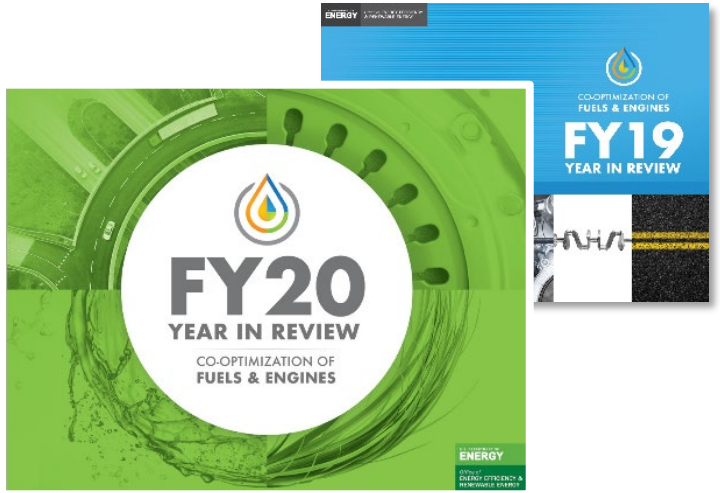
ACI (FY21, FY22 wrap up)

- Gasoline range blendstock identification and production, materials compatibility, ACI focused kinetics
- Fuel property effects on various gasoline ACI strategies including spray effects
- Fuel property effects on diesel multimode ACI
- Kinetics mechanism development
- Based on fuel properties identify most promising blendstocks

Co-Optima information online

- **Summary year-in-review documents**
  - **The best resource for a high-level overview of accomplishments**
  - **FY16-FY20 available online**

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



- **Searchable publication database**

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

- **VTO Annual Merit Review Presentations** (Fuels and Lubricants)

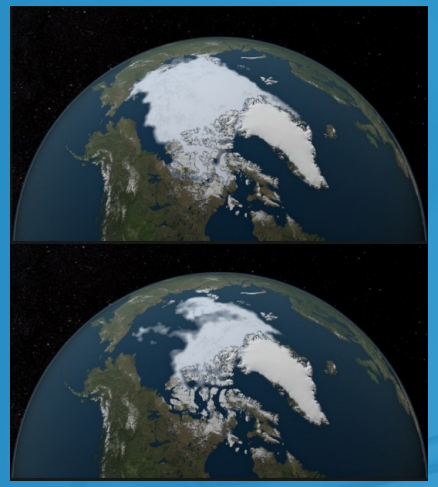
https://www.energy.gov/eere/vehicles/annual-merit-review-presentations

- **BETO Peer Review Presentations**

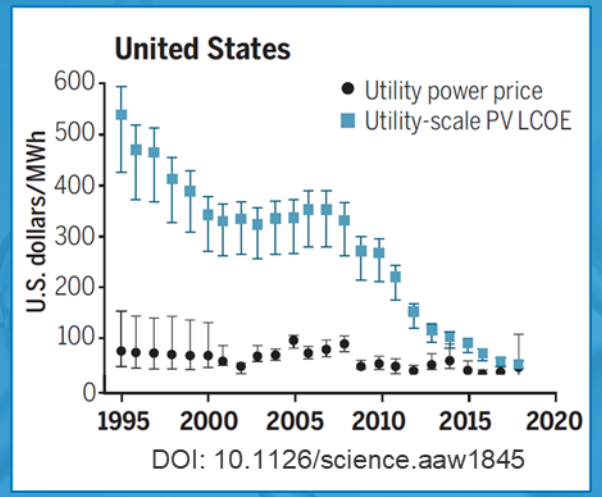
https://www.energy.gov/eere/bioenergy/downloads/2019-project-peer-review-co-optimization-fuels-and-engines

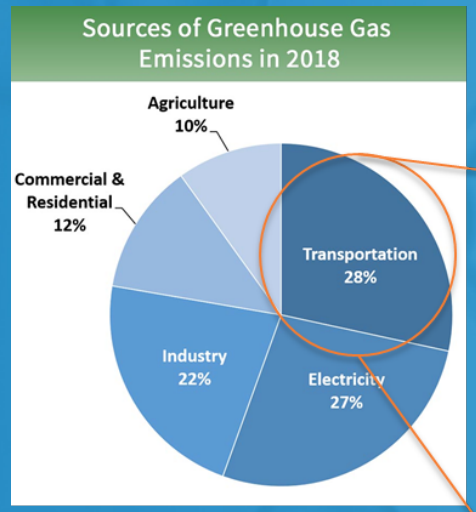
How the world has changed since 2016

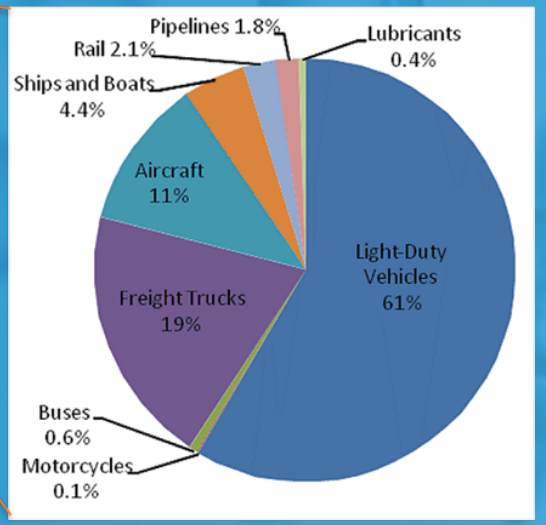
- New awareness of policy makers, industry, and the public of the danger of climate change
- Realization that zero net carbon emissions will be required
- Dramatic reductions in the cost of renewable electricity
- Transportation has become the largest GHG emitting sector
- Momentum to electrify the global LD auto and motorcycle fleet, transit buses and potentially other MD/HD applications



nasa.gov

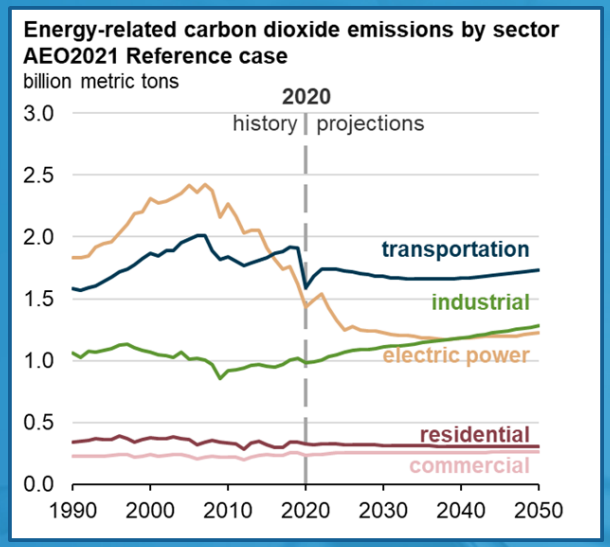


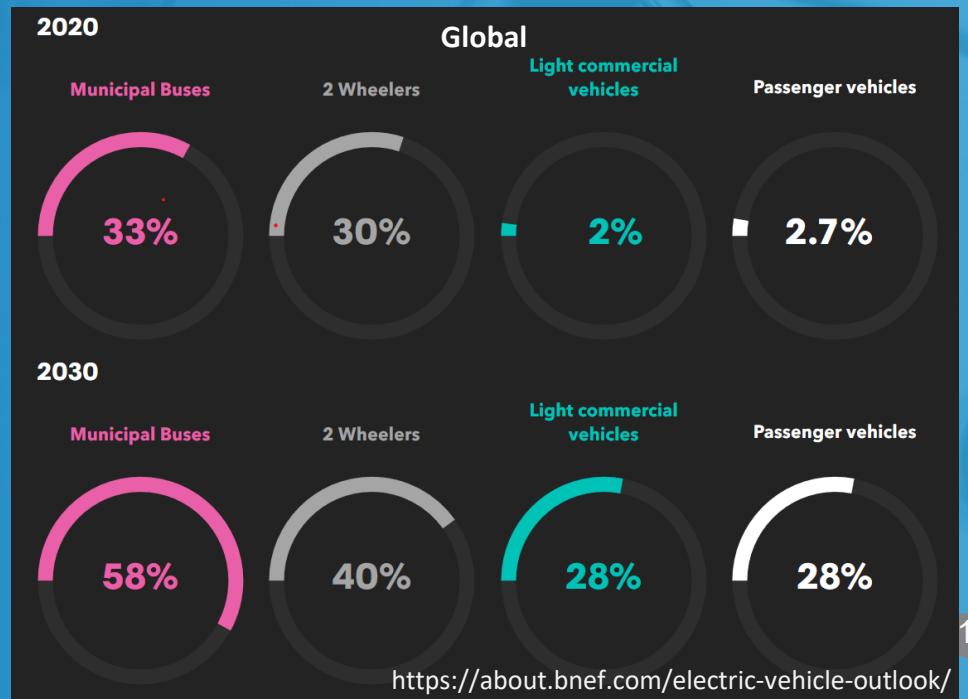




How the world has changed since 2016

- New awareness of policy makers, industry, and the public of the danger of climate change
- Realization that zero net carbon emissions will be required
- Dramatic reductions in the cost of renewable electricity
- Transportation has become the largest GHG emitting sector
- Momentum to electrify the global LD auto and motorcycle fleet, transit buses and potentially other MD/HD applications



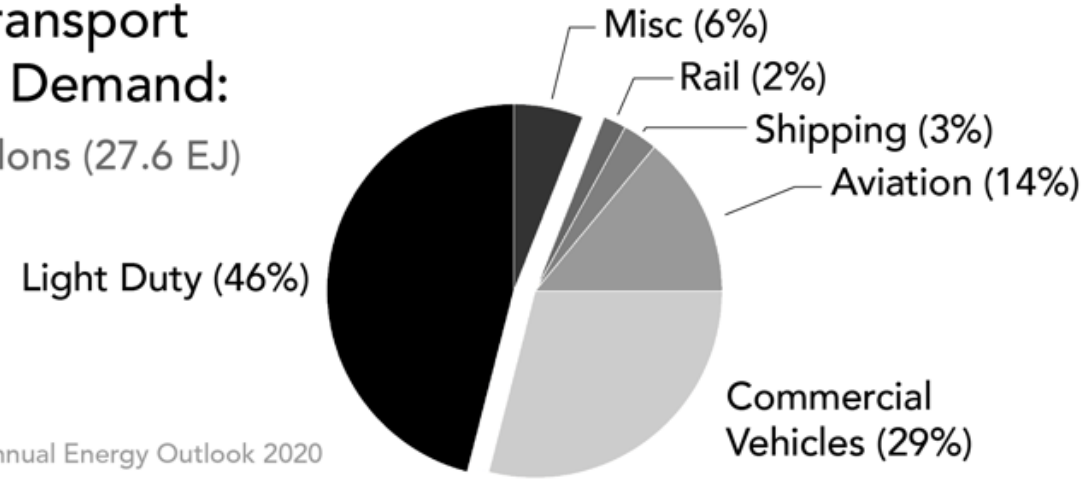


https://about.bnef.com/electric-vehicle-outlook/

The Real Challenge: Low-Carbon Fuels for Large Vehicles

2050 Transport Energy Demand:

190 B gallons (27.6 EJ)



Source: EIA Annual Energy Outlook 2020

"Hard to electrify" transportation segment represents almost half of all demand in 2050

Total demand: 82 billion gallons/year (11.9 EJ)

Benefits of low-carbon liquid fuels

- Early decarbonization of the existing vehicle fleet (LD, HD, …) using existing infrastructure
  - Expanding ethanol, biodiesel, and renewable diesel production and consumption in the near term
- Supports a just and inclusive transition to zero carbon
- Supports rural economy dependent on food and biofuel production
- Potentially only option – or lowest cost option – for largest vehicles

Realizing the potential from Co-Optima for decarbonization

- Highest impact with MD/HD vehicle focus
  - Learn to achieve net-zero criteria pollutants
- Reduce fuel carbon intensity while moving to larger scale
- Increase blend level up to 100%
- Overcome fuel adoption barriers
  - Fuel quality standards
  - Regulatory compliance
  - Engine manufacturer concerns
  - Multimedia assessment

Net-zero-carbon fuel development

Leverage Co-Optima work, extending GHG reduction target from 60% to net zero

Expand scope to include potential e-fuel candidates

Net-zero criteria and GHG emissions

Develop ducted fuel injection for soot-less operation

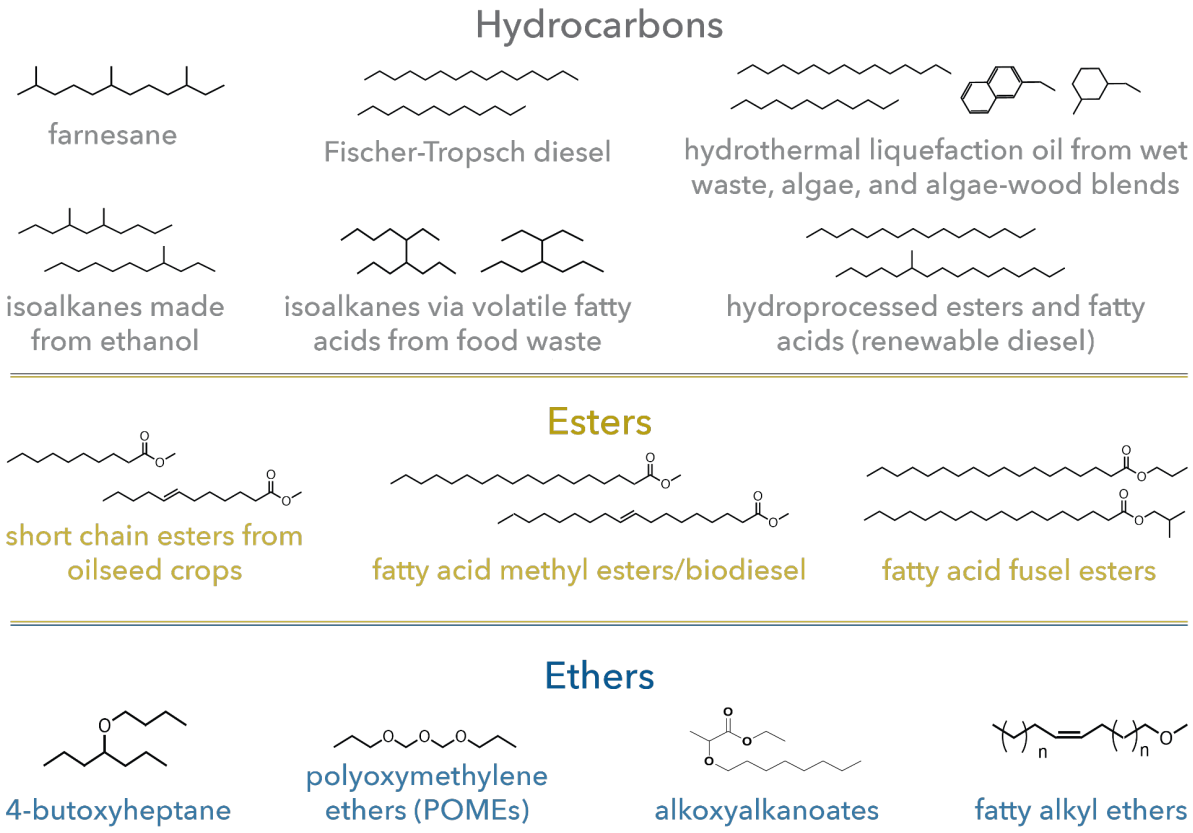
Develop improved emission control systems for lean NO_x and low-temperature oxidation

A first step ….

Expanding Adoption of Biomass- and Waste-Derived Fuels for Medium- and Heavy-Duty Ground Transportation

Replace high-net-carbon fuels with a diverse set of low or zero-net-carbon emissions liquid fuels

- *Beyond volumes available from currently used fats and oils feedstocks*
- *Improving efficiency has smaller impact but critical for reducing cost of ownership*



A first step… addressing barriers

- ***Technical adoption barriers for esters and ethers as diesel fuels***:
  - Current ASTM standards limit ester blending to 20 vol%, there are no standards for ethers
  - Limited data on high level ester blends, ethers are new to the diesel fuel market
  - Incremental scale up of production processes to reduce risk and provide fuel for evaluation
- ***Establish gasoline-boiling-range fuels for MD/HD***:
  - For MD and smaller HD vehicles SI engines may provide a lower cost path to criteria emissions compliance, and with fuels like 100% renewable E85 in optimized engines could approach the efficiency of diesel.
  - Longer term, GCI engines may provide high efficiency and low criteria pollutants with a more diverse set of fuels
- ***Market and regulatory barriers:***
  - Early engagement with OEMs and ASTM
  - Discuss with stakeholders such as CRC, RFA, Growth Energy, and NBB to identify cost-shared collaborations
  - Present annually to EPA and CARB

Capstone webinar series

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

Chuck 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?

Avantika Singh
National Renewable Energy 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?

Troy Hawkins
Argonne National 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 Laboratories

Daniel Gaspar
Pacific Northwest National Laboratory

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

Acknowledgements

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

Michael Berube
Deputy Assistant Secretary for Transportation

Valerie Reed
Acting Director, Bioenergy Technologies Office (BETO)

Alicia Lindauer
Technology Manager, BETO Bioenergy Analysis & Sustainability

David Howell
Acting Director, Vehicle Technologies Office (VTO)

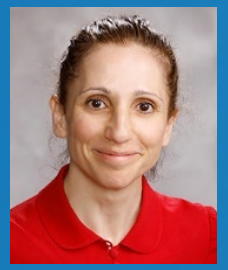
Gurpreet Singh
Program Manager, VTO Advanced Engine and Fuel Technologies

Kevin Stork and Michael Weismiller
Technology Managers, VTO Advanced Engine and Fuel Technologies

Contact

Bob McCormick
National Renewable Energy Laboratory
robert.mcccormick@nrel.gov

Dan Gaspar
Pacific Northwest National Laboratory
daniel.gaspar@pnnl.gov



Anthe George
Sandia National Laboratories
angeorg@sandia.gov

Robert Wagner
Oak Ridge National Laboratory
wagnerrm@ornl.gov