Co-Optima Capstone Webinar Series

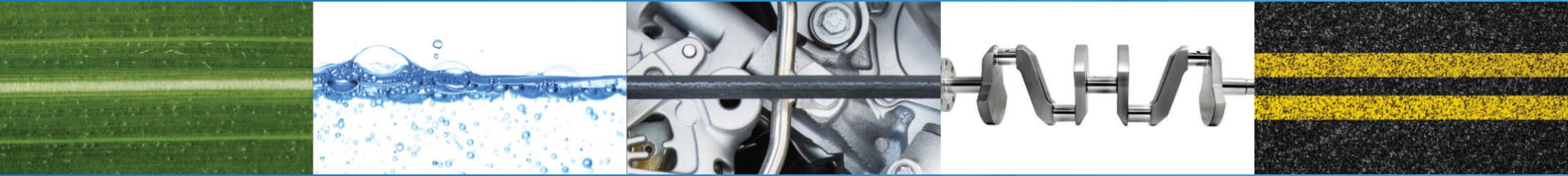
Co-Optimization of Fuels & Engines: Past, present, and future—what did we learn and where do we go next?

Daniel Gaspar – Pacific Northwest National Laboratory
Robert Wagner – Oak Ridge National Laboratory
On behalf of 200+ laboratory, university and industry Co-Optima researchers

September 30, 2021

CO-OPTIMIZATION OF FUELS & ENGINES

better fuels | better vehicles | sooner



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

Last in the Co-Optima 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

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?

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 & Engines: Past, present, and future—what did we learn and where do we go next?

Robert Wagner
Oak Ridge National Laboratory

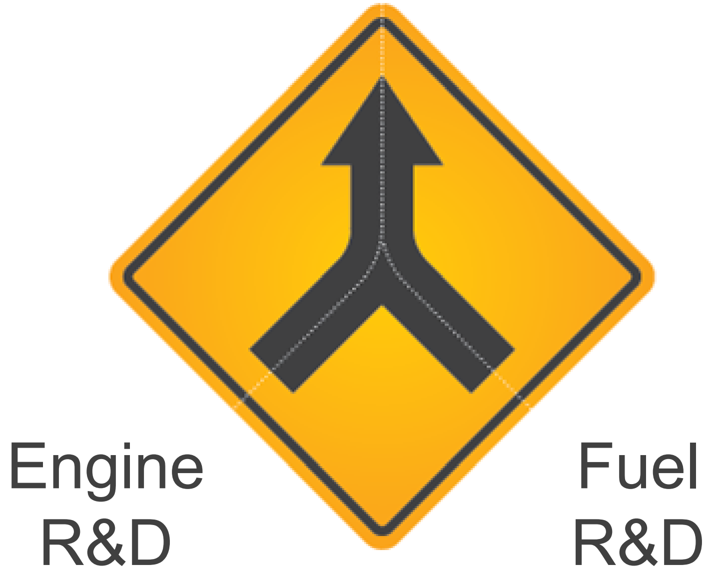
Daniel Gaspar
Pacific Northwest National Laboratory

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

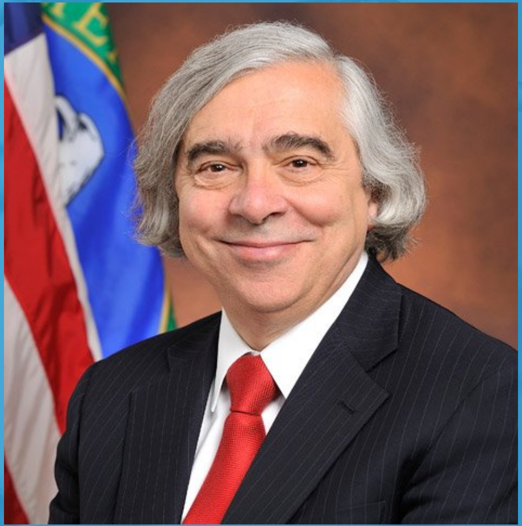
This is the story of how Co-Optima made the world better

- Where did we start?
- Where are we now?
- Where do we go from here?

Better fuels. Better engines. Sooner.



Where were we back in 2014?



Dr. Ernest Moniz, U.S. Secretary of Energy, 2013-2017

We were motivated by the
DOE Quadrennial Technology Review

"… reliance on oil is the greatest immediate threat to U.S. economic and national security, and also contributes to the long-term threat of climate change."

The laboratories came together at the DOE Big Idea Summit …

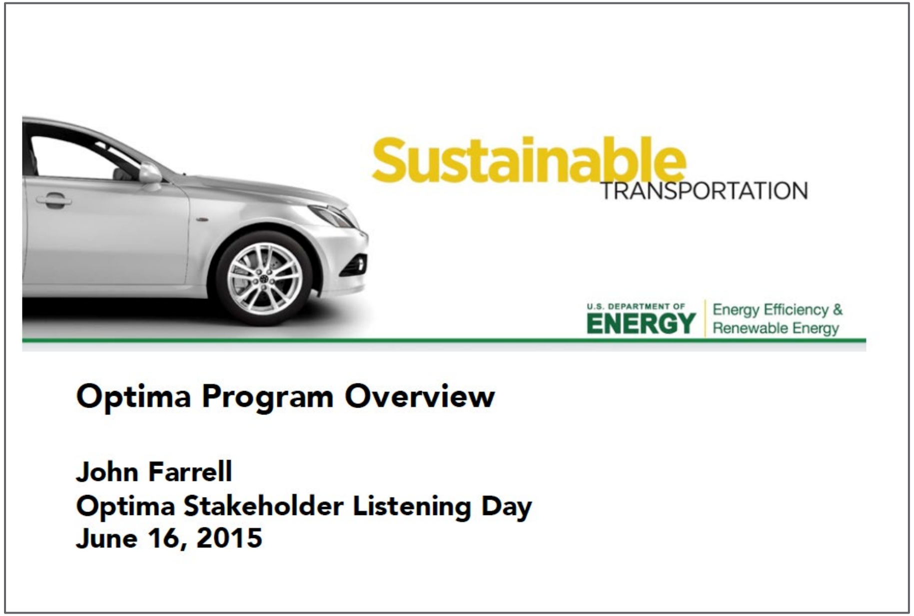
Opportunity to strategically align multiple national laboratories and DOE offices

… to make a difference by changing fuel and engine research

- Accelerate innovation and increase transportation sustainability
- Identify fuel-engine combinations and technology options to increase efficiency and reduce emissions

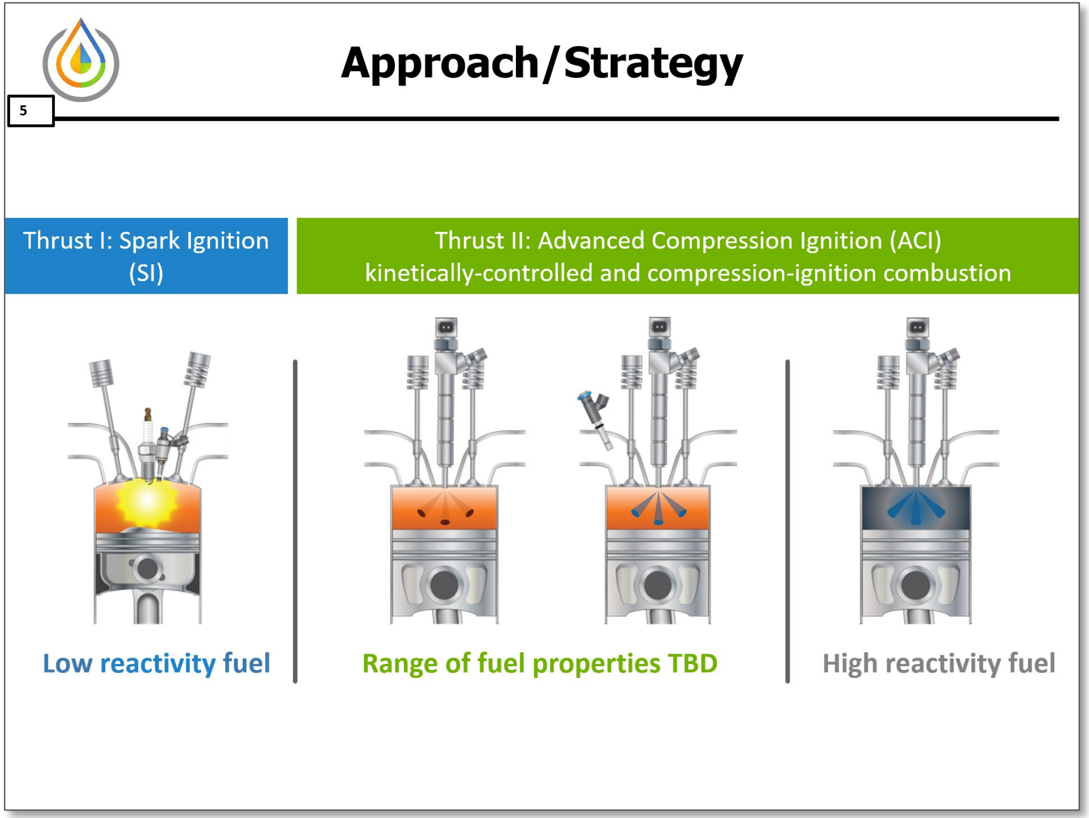
Nine national laboratories and two DOE offices came together

We engaged with stakeholders to guide our planning



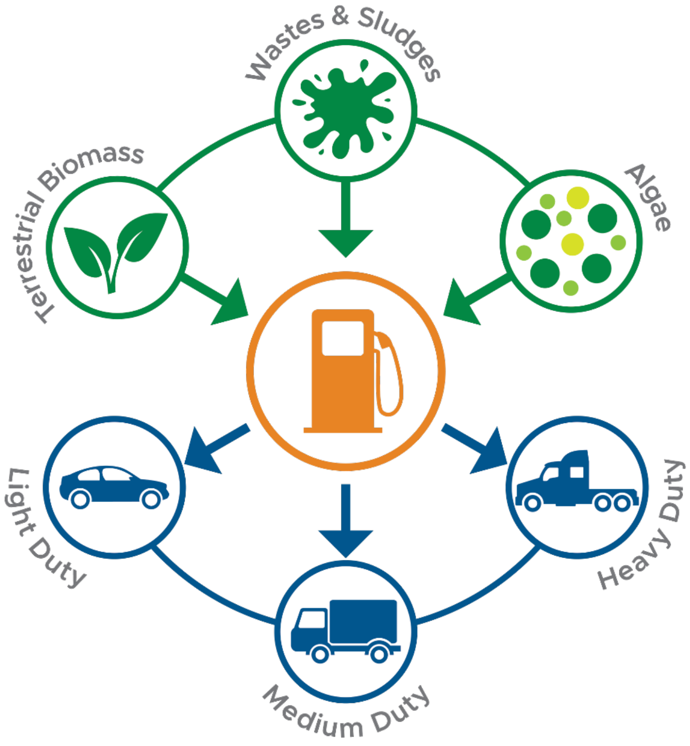
Original approach focused on combustion strategies

- Research thrusts focused on spark-ignition and compression-ignition combustion and fuels
- Focus was reworked based on industry recommendations



Scope was defined based on stakeholder input and DOE priorities

- Focus only on liquid fuels
- Identify blendstocks to blend into petroleum base (up to 30% by volume)
- Identify fuel properties that optimize engine performance, independent of composition
- Consider only non-food-based biofuel feedstocks
- Assess well-to-wheels emissions (greenhouse gases, water, etc.)
- Consider hybridized and non-hybridized powertrain solutions
- Provide data, tools, and knowledge to stakeholders



Structure was reworked based on industry input

Light Duty (LD)

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

Medium/Heavy Duty (MD/HD)

- **Near-term. MD/HD mixing-controlled compression ignition (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

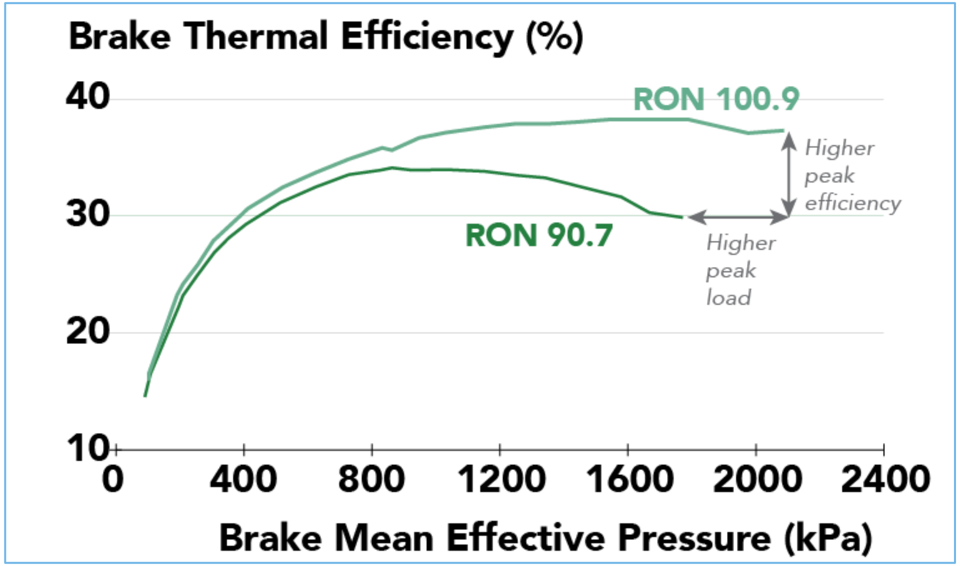
Objectives included **improving efficiency** and reducing GHG

Light-duty

Aiming for 10% based on known potential for higher efficiency

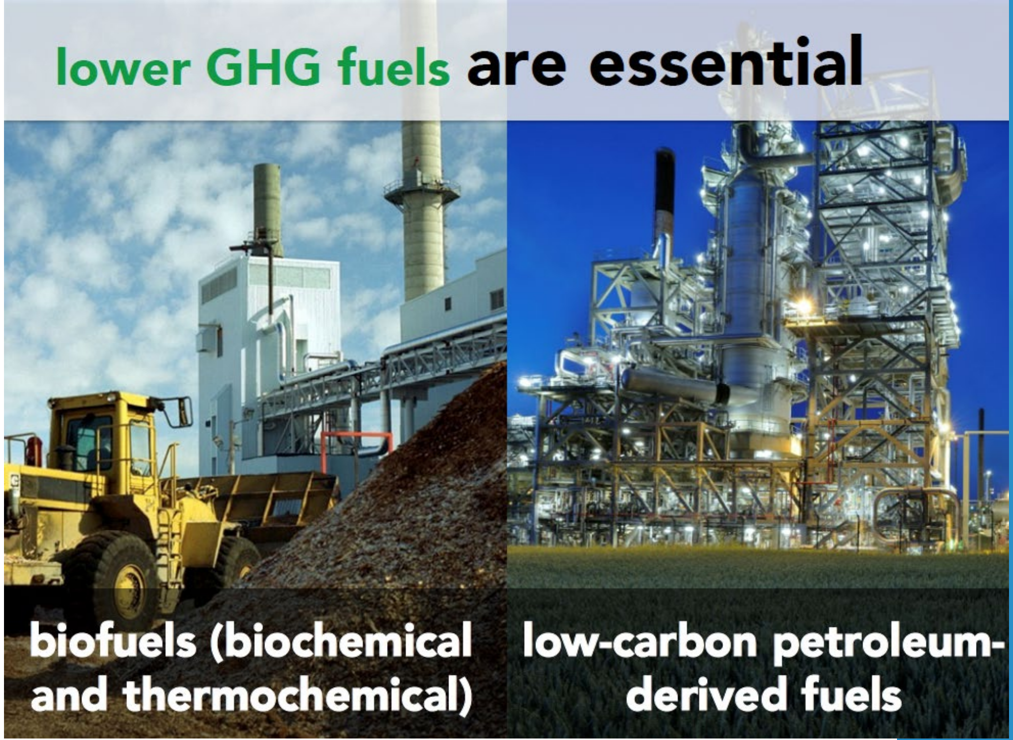
Medium/Heavy-duty

Aiming for diesel-like efficiency with lower emissions



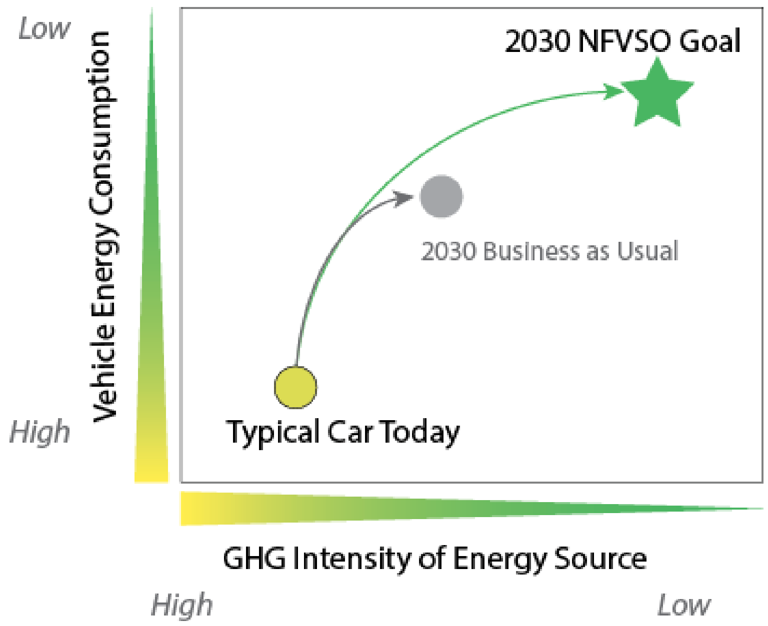
Engine: Ford Ecoboost 1.6L 4-cylinder, turbocharged, direct-injection, 10.1 CR
Source: C.S. Sluder, ORNL

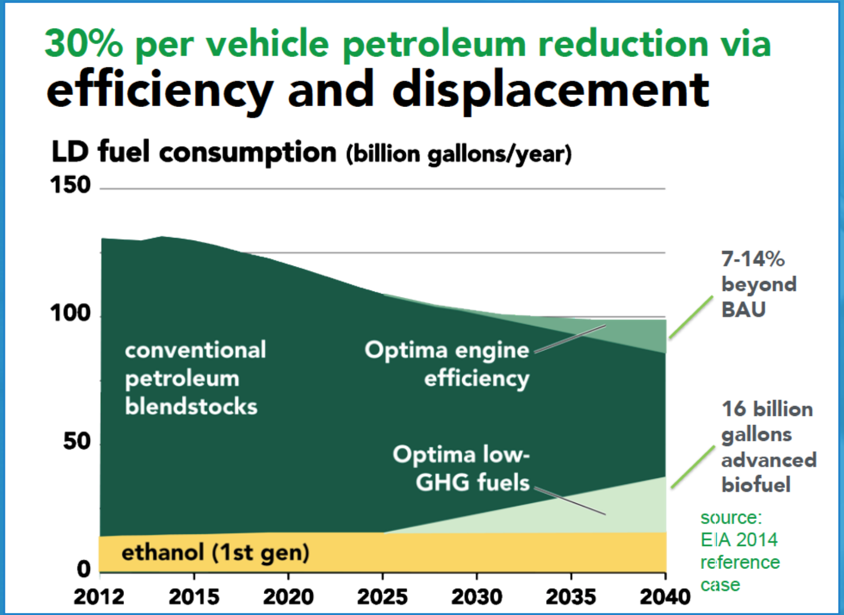
Objectives included improving efficiency and **reducing GHG**



Multiple pathways possible to reduce greenhouse gas (GHG) emissions

Potential for 30% per vehicle petroleum reduction

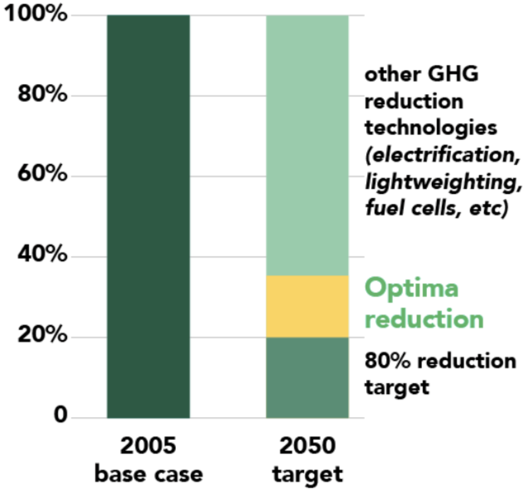




Potential for 30% per vehicle petroleum reduction

9-14%

GHG reduction beyond BAU

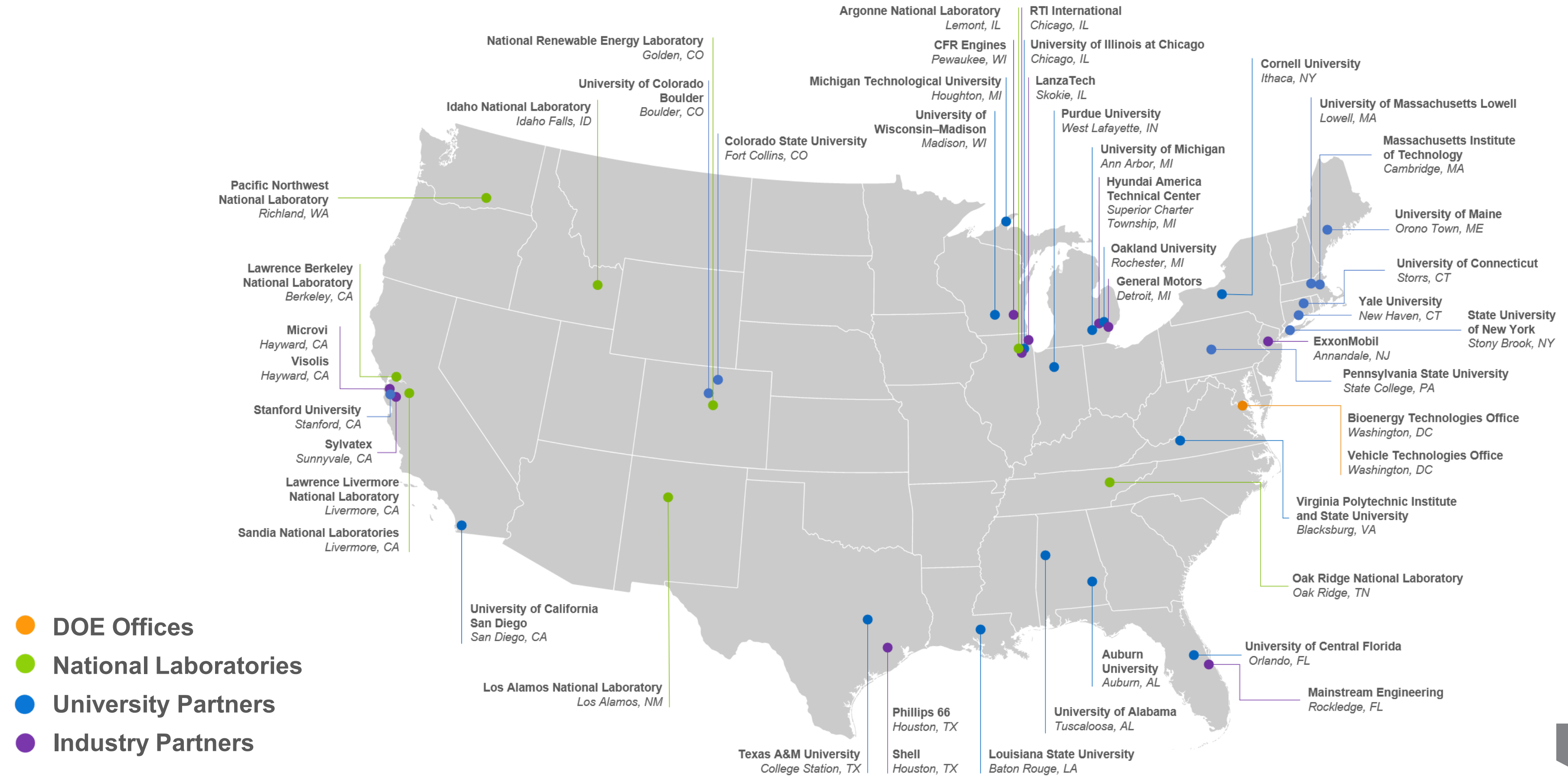


BAU = business as usual

This was considered very aggressive at the time but is not enough anymore

The team expanded from the original nine labs and two offices …

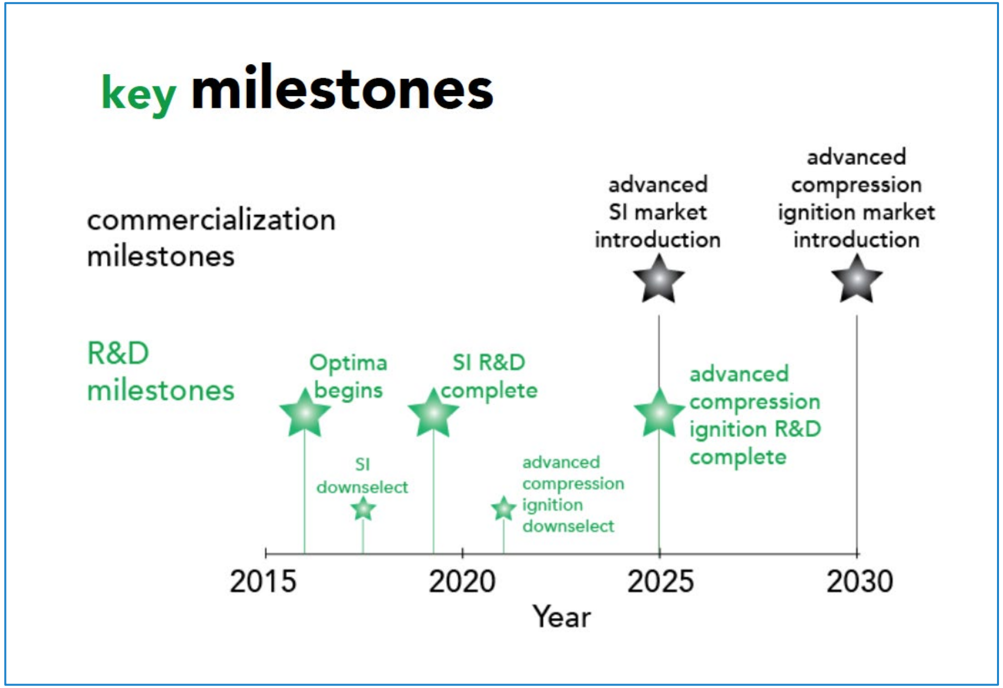
… to include universities and industry



Timeline and objectives also changed from original plan

Original plan was 10-year initiative with a path to market

Plan was accelerated to a 6-year timeline and the path to market was deemphasized to focus on science



Key Takeaways

So…how did we do?

OUTCOMES Co-Optima largely met its goals

Light Duty

- 10% fuel economy gain over 2015 baseline
- Potential *additional* 9-14% gain via multimode approaches
- Merit function tying fuel properties to fuel economy
- Top 10 sustainable blendstock options offering performance gains (RON, S, HOV)

Medium and Heavy Duty

- Potentially lower-cost path to reduced engine-out criteria emissions
- Top 13 sustainable blendstock options with performance advantages (soot, cetane number, operability)
- >4% fuel economy gain and lower emissions via ACI

Crosscutting

- Blendstock options to decrease GHGs by 20%+ in the near term for 30% renewable blends
- Potential economic drivers to increase adoption
- New tools, extended and linked simulation approaches
- Extensible screening methodology

RON = research octane number; S = sensitivity; HOV = heat of vaporization

Notable Outcomes

- Low-carbon biofuels could be produced at near-competitive prices.
- Changes in engine design and operation coupled to fuel property changes can improve efficiency.
- Biofuels can reduce GHGs for cars and trucks already on the road, while advanced engines have additional NO_x/PM benefits.

NO_x = nitrogen oxide; PM = particulate matter

OUTCOMES Merit function points the way for LD

$$Merit = 100 * \frac{\eta - \eta_{ref}}{\eta_{ref}}$$

Octane Index Terms

$$= \frac{(RON[-] - 91)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})} - K[-]\frac{(S_{Octane}\,[-] - 8)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})}$$

Heat of Vaporization on Knock Mitigation

$$+ \frac{0.085\left[\frac{kJ}{kg}\right]^{-1} \cdot \left(\frac{HoV\left[\frac{kJ}{kg}\right]/(AFR[-]+1) - 415[kJ/kg]}{14.0[-]+1}\right)}{1.6 + 0.3 * H(PMI - PMI_{LSPI,crit})}$$

Other Combined Heat of Vaporization

$$+ \frac{HoV[kJ/kg]/(AFR[-]+1) - (415\left[\frac{kJ}{kg}\right]/14.0[-]+1)}{15.3\left[\frac{kJ}{kg}\right]}$$

Flame Speed

$$+ \frac{(S_L[cm/s] - 46[cm/s])}{5.4\left[\frac{cm}{s}\right]}$$

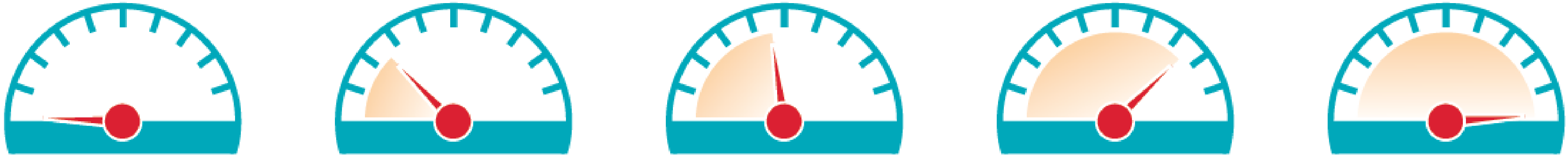
Particulate Emissions

$$- H(PMI - 1.6)[0.7 + 0.5(PMI - 1.4)]$$

Catalyst Light-Off

$$+ 0.008[°C]^{-1}(T_{c,90,conv}\,[°C] - T_{c,90,mix}\,[°C])$$

Fuel properties can lead to higher efficiency

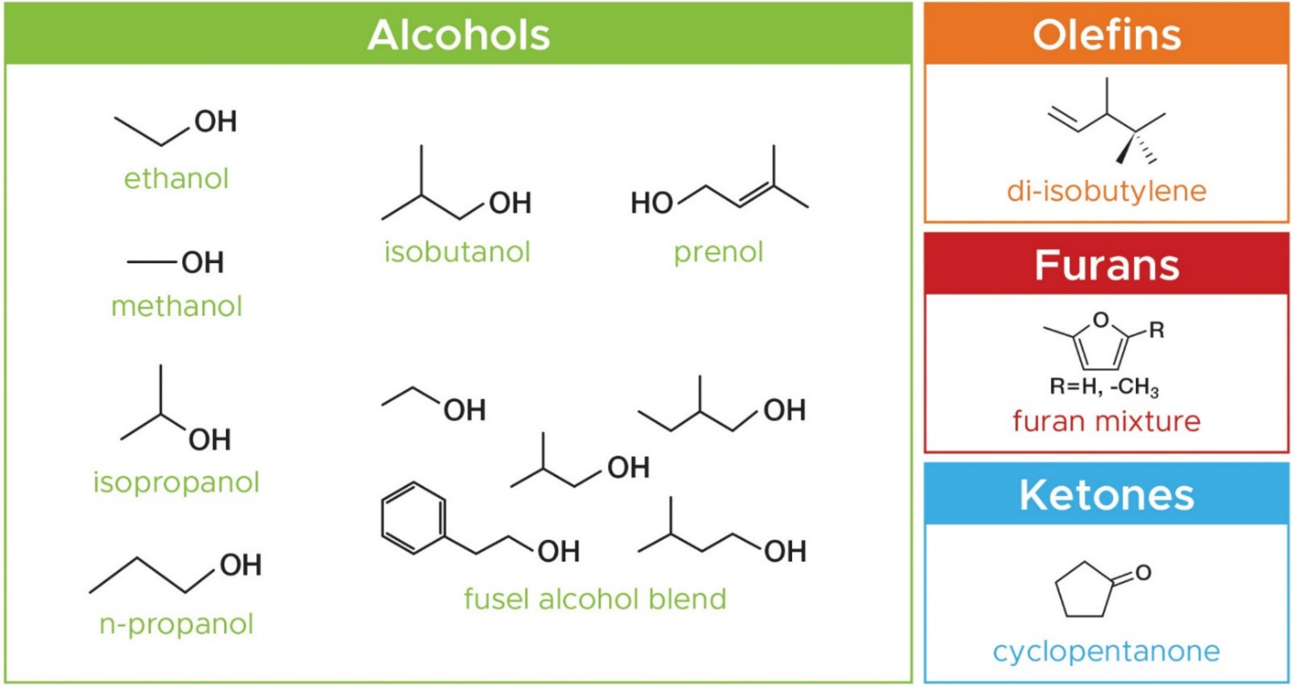


0%	2.5%	4.4%	7.5%	10%
91 RON	95 RON	98 RON	98 RON	102 RON
S=8 Baseline	S=8	S=8	S=12	S=12
CR = 9.7 Baseline	CR=11	CR=12	CR=13.7	CR=15

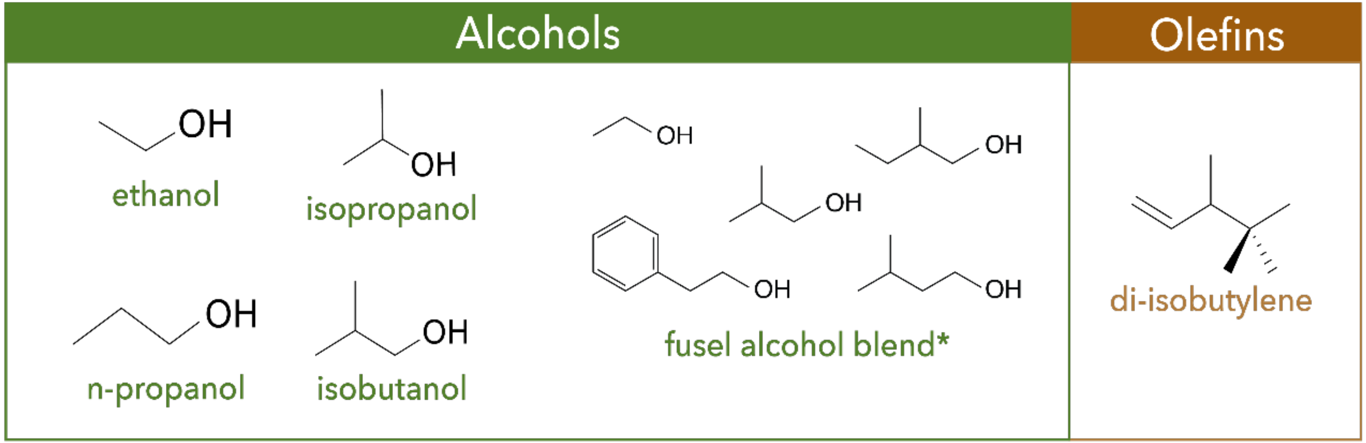
- Blendstocks which increase RON and S enable higher compression ratio (CR)
- Higher CR increases efficiency

OUTCOMES There are many blendstock options

Blendstocks with highest merit function score blend synergistically



OUTCOMES Six have highest potential, lowest entry barriers

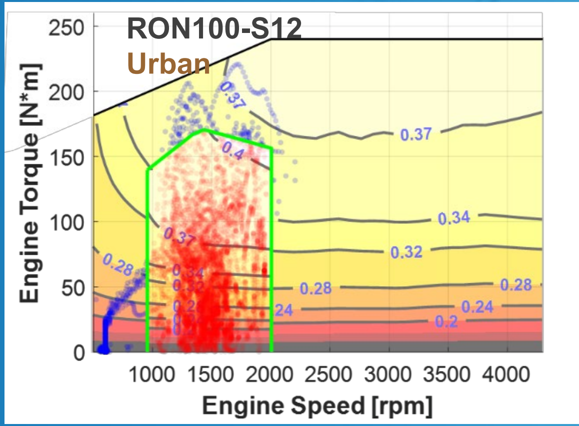


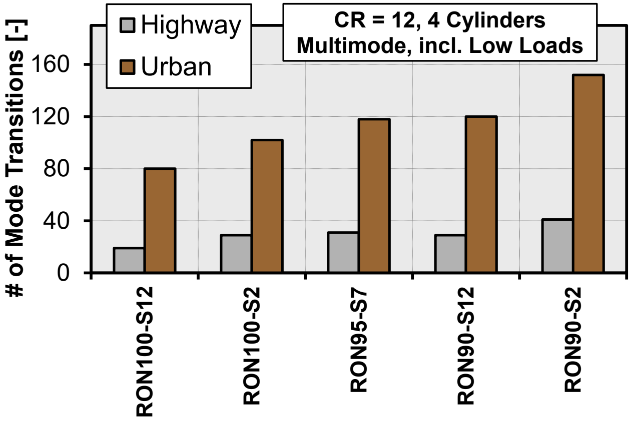
*Fusel alcohol blend: 57% isobutanol, 15% phenyl ethanol, 12% 3-methyl-1-butanol, 10% ethanol, 6% 2-methyl-1-butanol

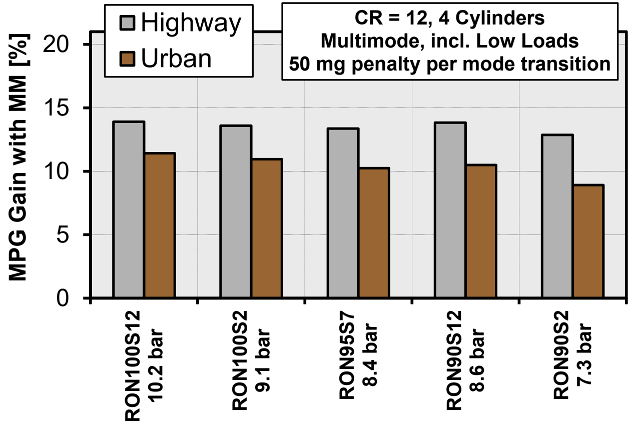
- Ethanol, isobutanol, and di-isobutylene allowed in gasoline now
- Other alcohols are chemically similar to ethanol and isobutanol

OUTCOMES Multimode offers further fuel economy benefits

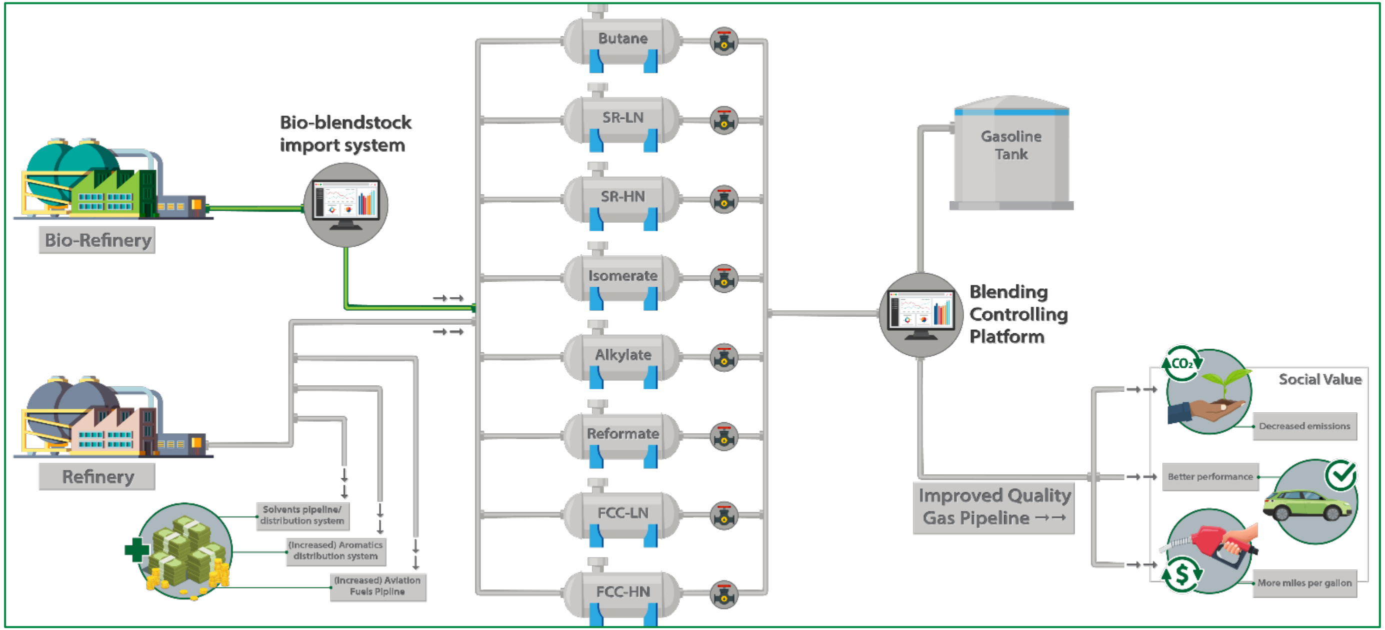
- Multimode operation offers 9%–14% MPG gains for highway and urban drive cycles
- Mode switching is most frequent for urban drive cycle
- Higher spark-assisted compression ignition (SACI) load limit of high-RON, high-S fuels provides efficiency benefits







OUTCOMES Gasoline bioblendstocks offer value during transition



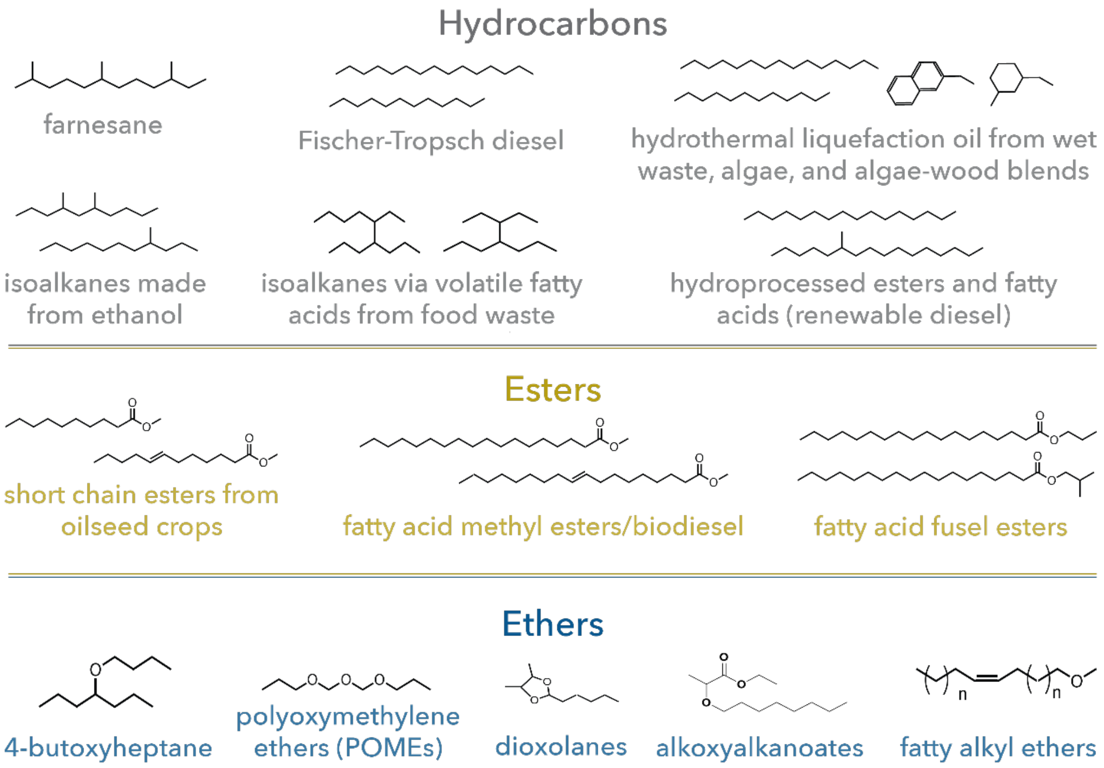
- Lower GHG emissions
- Multiple value streams to refiners
- Higher engine efficiency possible

OUTCOMES Screening identified 13 promising MCCI biofuels

Hydrocarbons
Lowest barriers to introduction

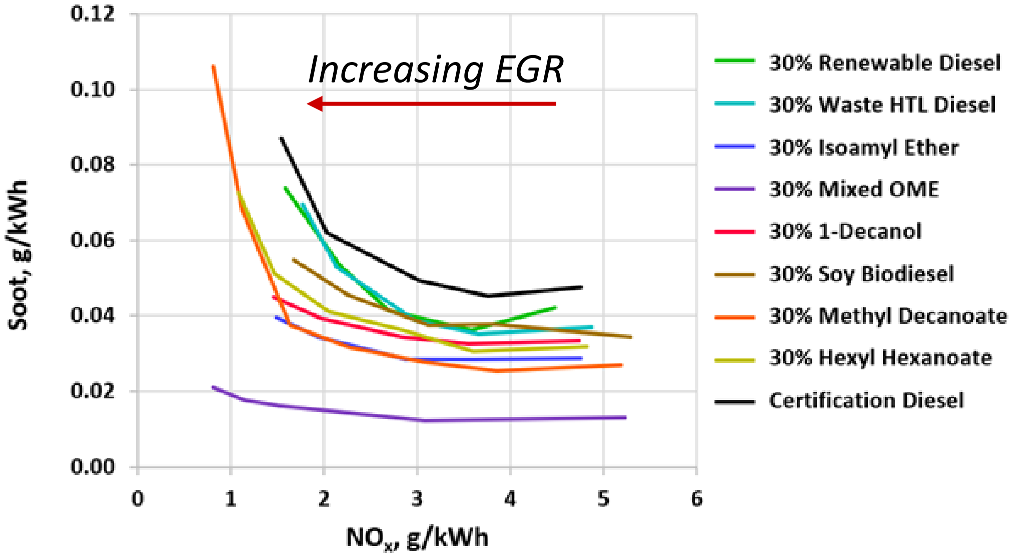
Esters
Some barriers to use at high blend levels

Ethers
Highest barriers to introduction



OUTCOMES Blendstocks reduced soot and NO_x

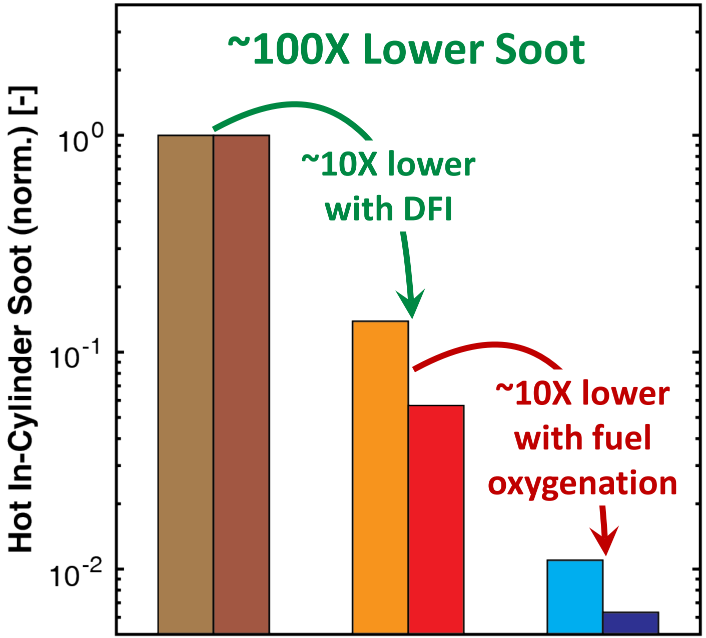
- All bioblendstocks resulted in lower soot
- Some blends tolerated higher levels of exhaust gas recirculation (EGR), leading to even lower NO_x



EGR tolerance = ability to maintain low soot @ high EGR

OUTCOMES DFI is synergistic with oxygenated fuels

Many low-net-CO_2 sustainable fuels are oxygenated



Conventional Diesel Combustion
- Diesel fuel, no EGR (21% O_2)
- Diesel fuel, moderate EGR (16% O_2)

Ducted Fuel Injection (DFI)
- Diesel fuel, no EGR (21% O_2)
- Diesel fuel, moderate EGR (16% O_2)
- Diesel fuel with 25 vol% oxygenate, no EGR (21% O_2)
- Diesel fuel with 25 vol% oxygenate, moderate EGR (16% O_2)

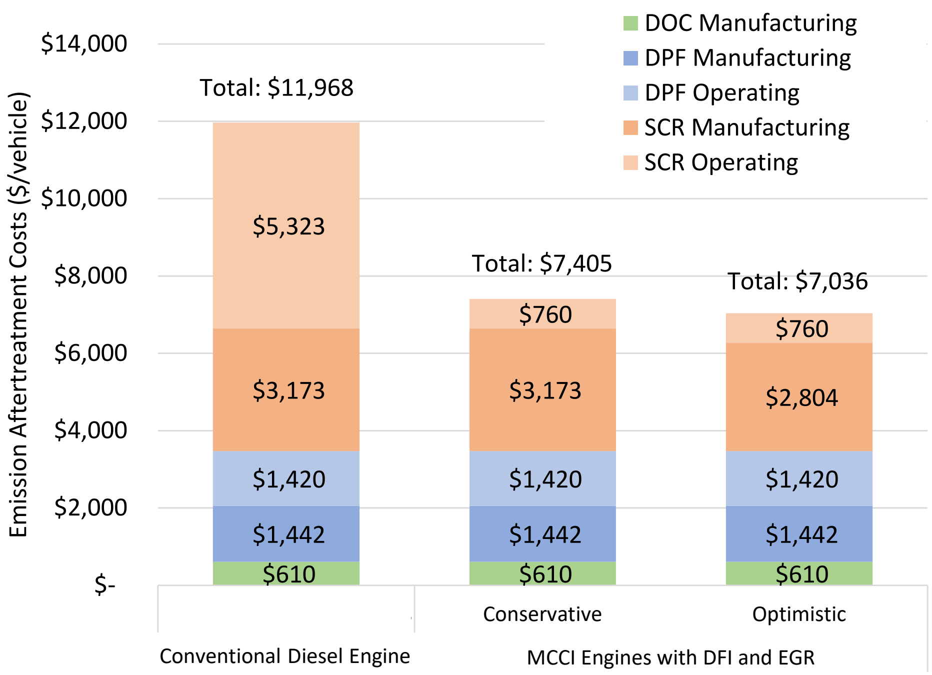
*Results for ~2.6 bar gross indicated mean effective pressure, 1200 rpm, steady state, 2-hole injector

See doi: 10.1016/j.jaecs.2021.100024 for details

OUTCOMES

DFI, biofuels could reduce NO_x, PM control costs

- >90% reductions in engine-out NO_x and PM
- $4,500-$5,000 lifetime cost reduction
    - Reduce use of exhaust fluid
    - Downsize selective catalytic reduction system

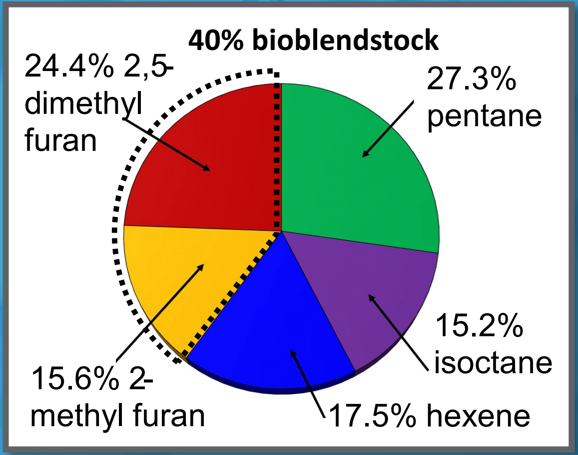


DFI = ducted fuel injection, DOC = diesel oxidation catalyst, DPF = diesel particulate filter, EGR = exhaust gas recirculation, SCR = selective catalytic reduction

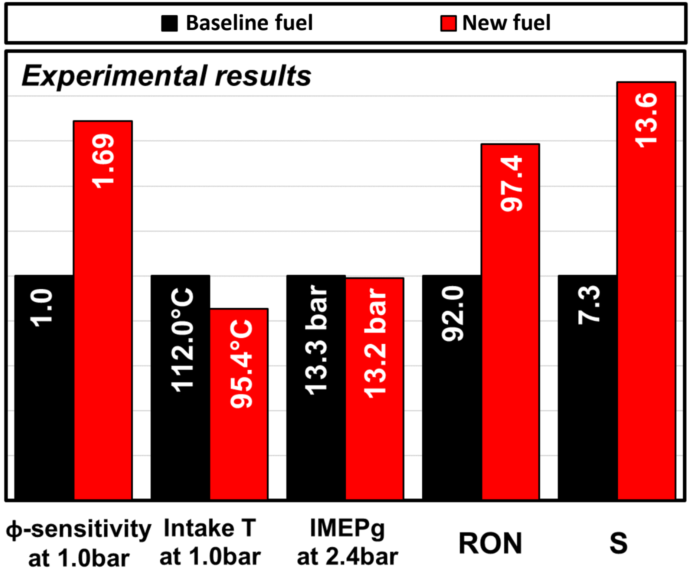
Advanced combustion approach for MD/HD

- Formulated better fuel, suitable for ACI and boosted-SI engines

New fuel with 40%$_{vol}$ furans



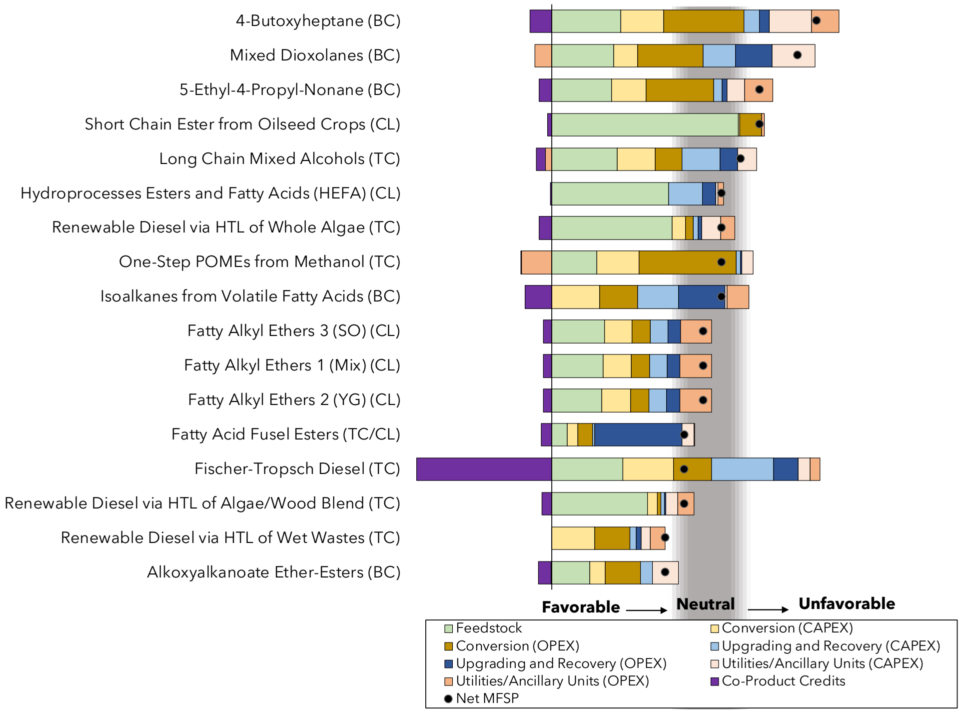
- It has high bioblendstock content and provides higher ϕ-sensitivity*, RON, and S



Intake T = intake temperature
IMEP$_g$ = gross indicated mean effective pressure
ϕ-sensitivity = measures how autoignition reactivity varies with air/fuel equivalence ratio; can correlate to efficiency, operability

OUTCOMES Reducing cost is a key challenge

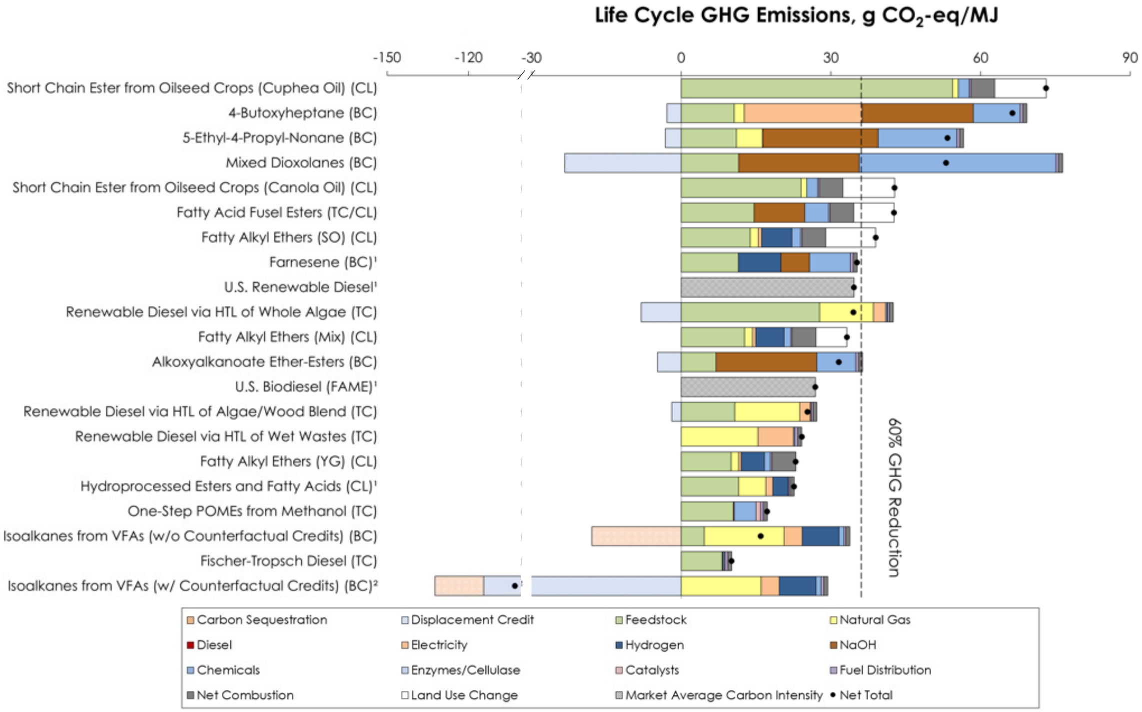
- Feedstock costs are major part of minimum fuel selling price (MFSP)
  - Waste pathways could reduce cost
- Conversion costs are highest for biochemical pathways
  - Caustic in pretreatment
  - Glucose in enzyme production
  - Low coproduct credits, upgrading, and recovery costs for most blendstocks



Cost breakdown of MFSP for selected MCCI bioblendstocks evaluated under Co-Optima. Costs broken down by overarching process hierarchies areas and further broken down to contributions by capital expense (CAPEX) and operational expenses (OPEX).

OUTCOMES There is potential for significant GHG reductions

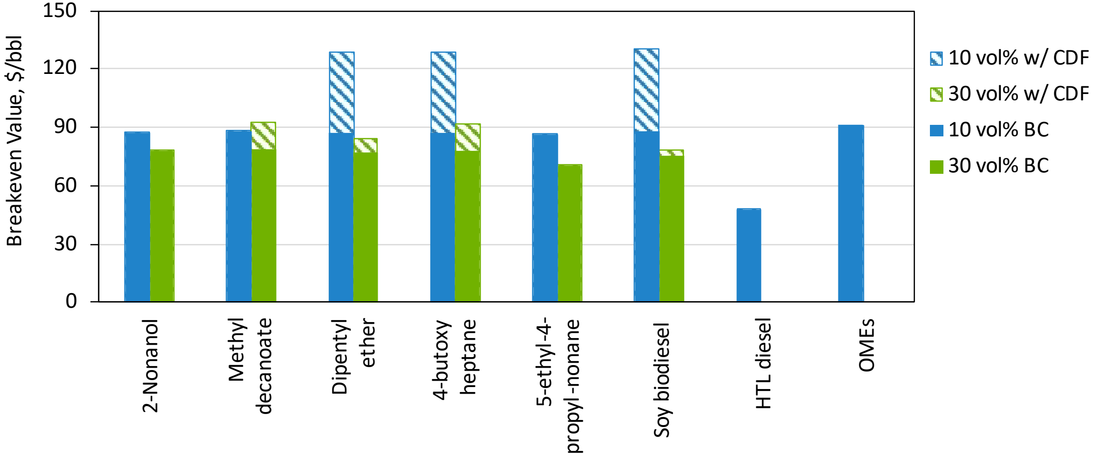
- …but they are not guaranteed for all biofuels
- Still room to improve GHG emissions
  - Feedstock production
  - Sodium hydroxide (NaOH) for feedstock pretreatment
  - Chemical inputs



Life cycle GHG emissions for MCCI blendstock candidates by GHG source. Blue dashed bars reflect credits associated with displacing emissions for co-products of bioblendstock production. Two blendstocks already on the market (U.S. Renewable Diesel and U.S. Biodiesel) were compared to nine additional candidates. The life cycle GHG emissions were evaluated using Argonne National Laboratory's 2020 GREET model.

OUTCOMES Diesel bioblendstocks could add value for refineries

WTI=$60/bbl, Year=2040, 11.5% Co-Optima blendstock in diesel



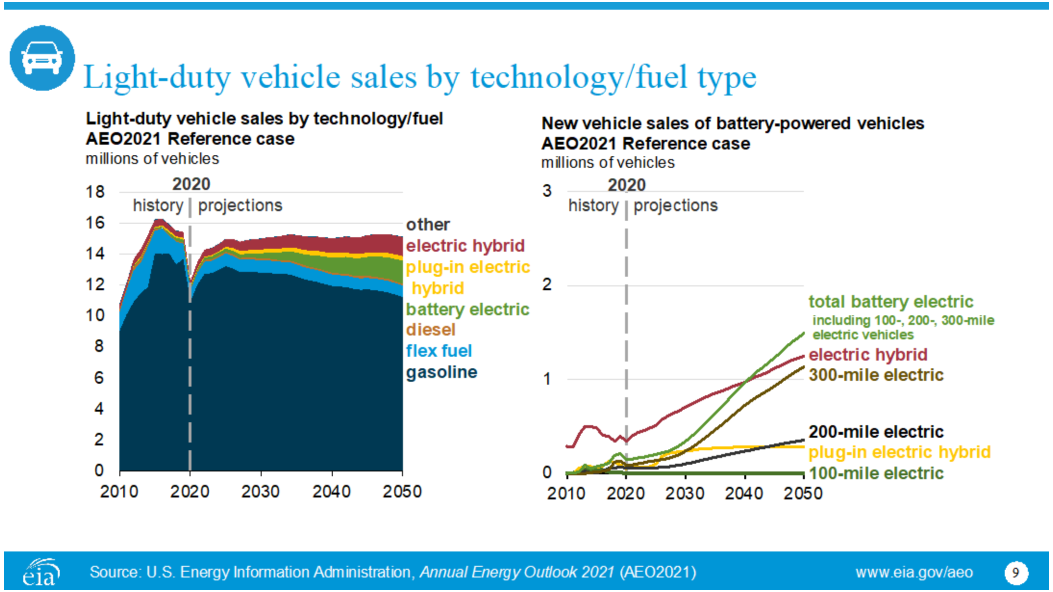
OMEs=oxymethylene ethers; ULSD=ultra-low sulfur diesel; CDF=California diesel fuel; WTI=West Texas Intermediate; BC=base case

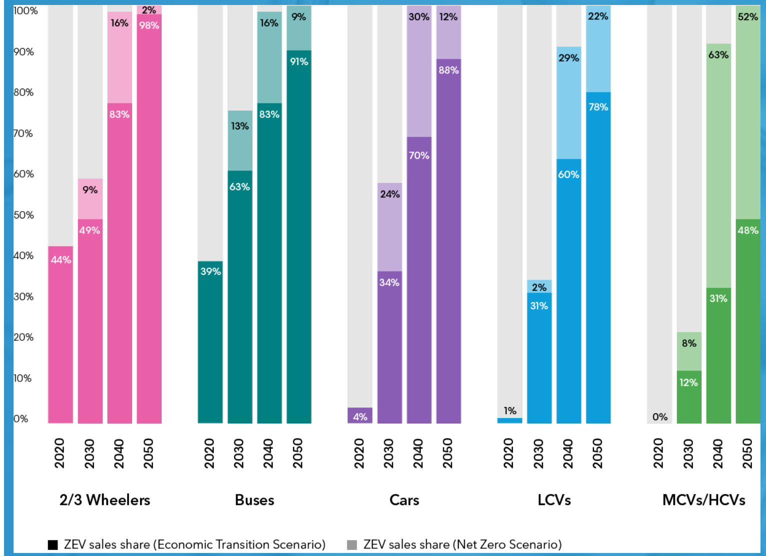
- Value is derived from low sulfur content in blendstock
- Where higher CN is required, additional value is provided by bioblendstocks with high CN
    - California
    - EU
    - India
    - China

Future R&D

- New ICEs and biofuels are part of the transition strategy (will be used in hard-to-electrify sectors longer).
- Biofuel scale-up, fit-for-purpose testing are needed.
- Focused engine technology development is needed to accommodate low carbon fuels and reduce emissions.

FUTURE R&D The world changes at an uncertain pace





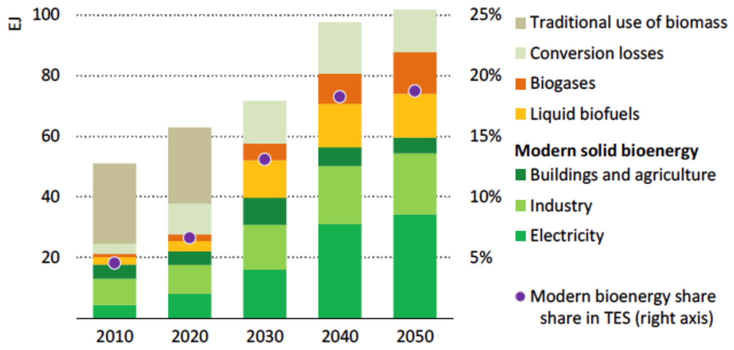
…and must change faster to address climate change

Solid bars = BNEF Economic transition scenario
Grayed color bars = BNEF Net Zero Scenario
Bars show actuals for 2020 and projections for 2030- 2050

Source: Bloomberg New Energy Finance EVO 2021

FUTURE R&D Address all transport modes to realize potential

Figure 2.20 ▹ Total bioenergy supply in the NZE

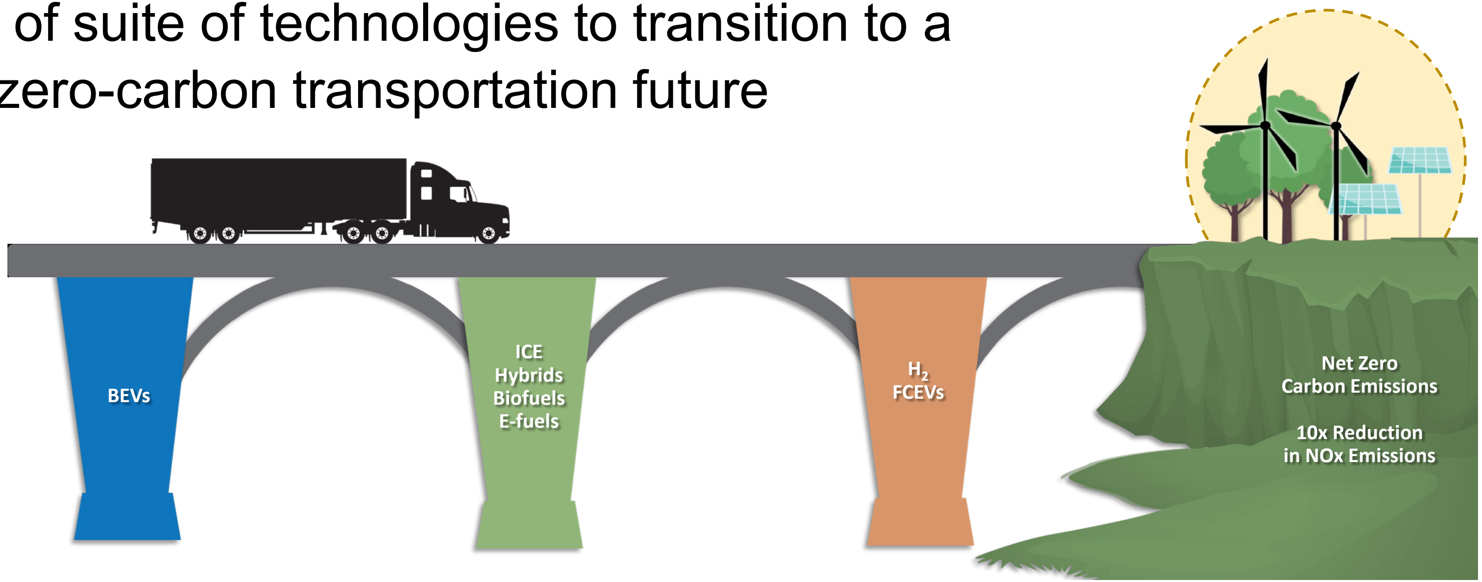


Modern bioenergy use rises to 100 EJ in 2050, meeting almost 20% of total energy needs. Global demand in 2050 is well below the assessed sustainable potential

- Importance of off-road transport modes (jet, marine, ground) is increasing
- Long-haul trucking will need liquid fuels for a longer period than LD vehicles
- Sustainable fuel supply must grow

This bridge will enable the energy transition

- Legacy internal-combustion engines (ICEs) will be on the road for decades
- Sustainable liquid fuels and hybrid ICEs can reduce carbon emissions of these vehicles *today*
- Part of suite of technologies to transition to a net-zero-carbon transportation future



Propulsion systems will evolve

- Propulsion choice will depend on application
- Electrify wherever possible, including hybrids

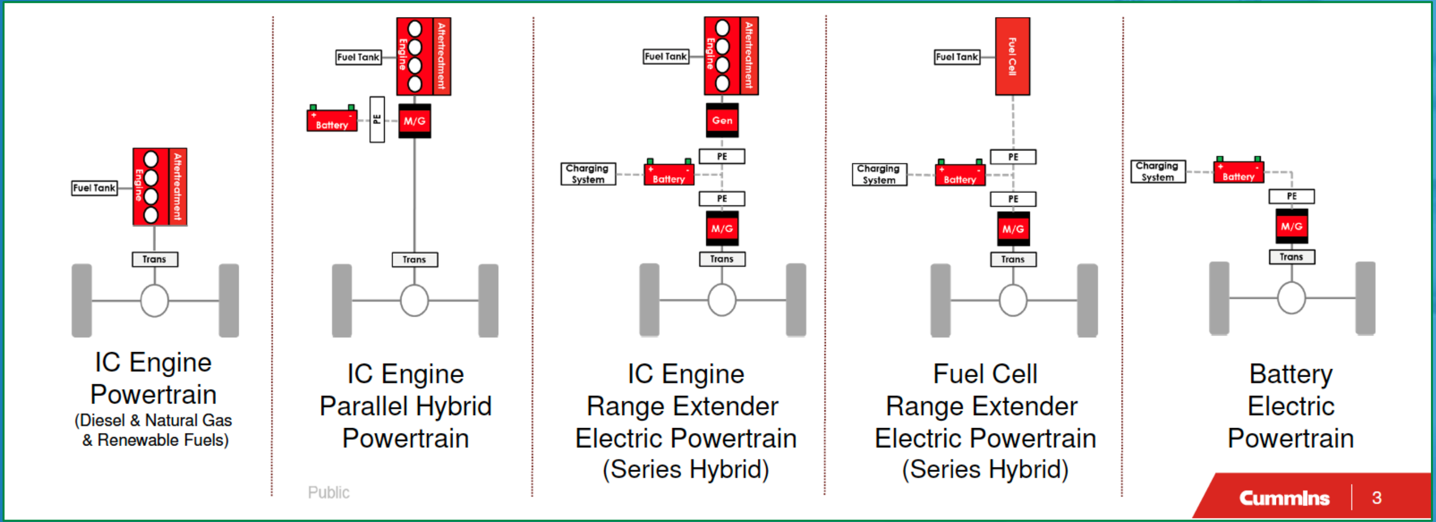
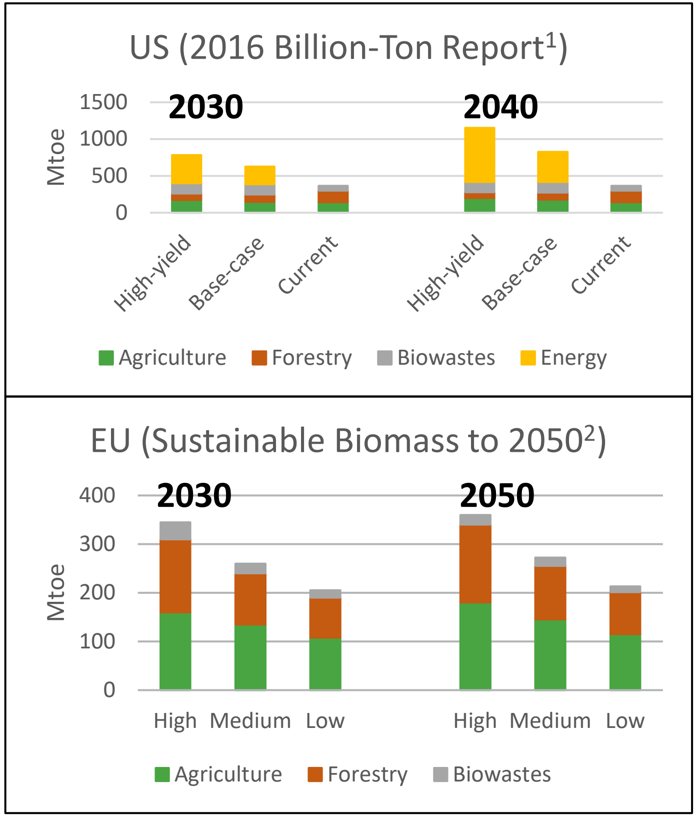


Figure courtesy of Cummins

FUTURE R&D Will there be enough biomass?



Mtoe = million or mega tonnes of oil equivalent

[1] DOE/ORNL *2016 Billion-Ton Report: Vol 1: Economic Availability of Feedstocks*. doi: 10.2172/1271651

[2] Imperial College London *Sustainable biomass availability in the EU, to 2050.* RED II Annex IX A/B. Panoutsou, C. and Maniatis, K.

- Most likely, yes, with the right investments
- U.S. can produce 60 bn gal/yr fuel from 1 bn ton biomass
- Electrification will liberate ethanol capacity for upgrading
- Europe has enough to cover all fuels & products
- Renewable hydrogen needed for mature thermochemical technologies

FUTURE R&D Overcome barriers to use of net-zero-carbon fuels

- 90-100% low-GHG fuels
  - Expanded supply at lower cost
  - Ensure fuels are fit-for-purpose
  - ASTM standards
  - OEM approval
- Engine modifications
  - Exploit improved and/or different properties
  - Determine changes needed to operate on fully sustainable fuels

MCCI Blendstock	Fluorocarbon	Fluorosilicone	Polyurethane	Epichlorohydrin	PVC/nitrile/ butadiene blends	Hydrogenated nitrile butadiene	Nitrile butadiene rubber
Renewable diesel							
Biodiesel							
Butylcyclohexane							
Mixed dioxolanes							
4-Butoxyheptane							
n-Undecane							
Methyl decanoate							
Hexyl hexanoate							
1-Octanol							
1-Nonanol							
2-Nonanone							
2-Pentanone							
TPMGE							

Suitable
Borderline
Unsuitable

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CAPSTONE WEBINARS Recordings at link below

MAR 25

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

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

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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 & 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

Additional Resources

energy.gov/fuel-engine-co-optimization

energy.gov/eere/bioenergy/co-optima-publications