Co-Optima Capstone Webinar Series

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

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner

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

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Overview

- The Challenge
- The Goal
- Key Takeaways
- Research Approach
- Notable Outcomes
- Next Steps

Better fuels. Better engines. Sooner.

Engine R&D

Fuel R&D

The Challenge

Maintain desirable attributes of diesel engines while achieving net-zero carbon, nitrogen oxides, and soot

BACKGROUND Motivation

Society needs **cost-effective**, **clean**, **low-carbon** powertrains for applications that require:

- Long range
- Rapid re-energizing
- Light weight
- Compact size

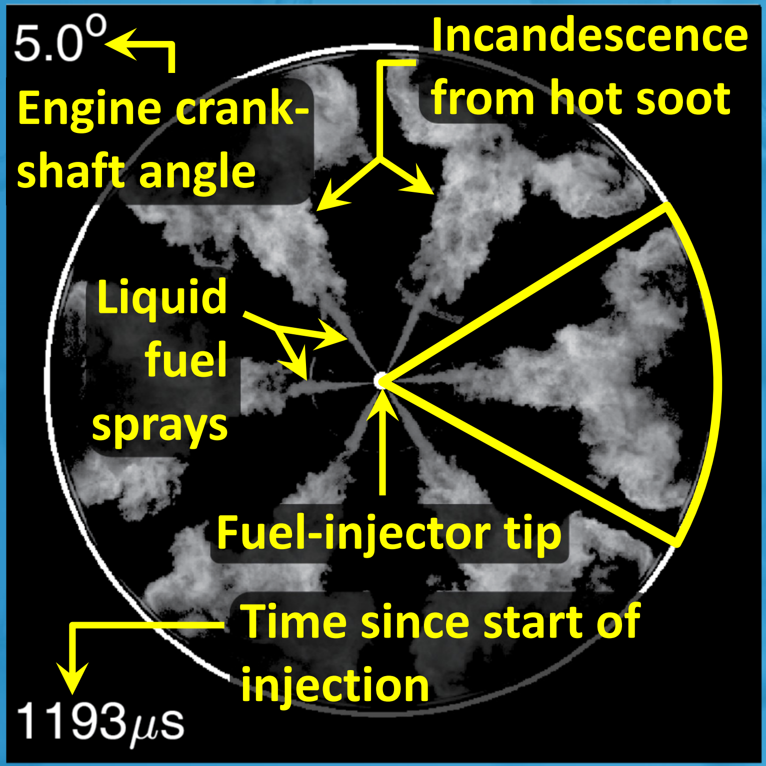
Potential solutions:

- **Electric motors** powered by
  - **Batteries** (cons: expensive, heavy, large)
  - **Fuel cells** (cons: expensive, low energy density of H_2 fuel, current high net CO_2)
- **Diesel engines** powered by
  - **Petroleum fuels** (cons: high net CO_2, toxic emissions)
  - **Sustainable fuels** (cons: toxic emissions, expensive)

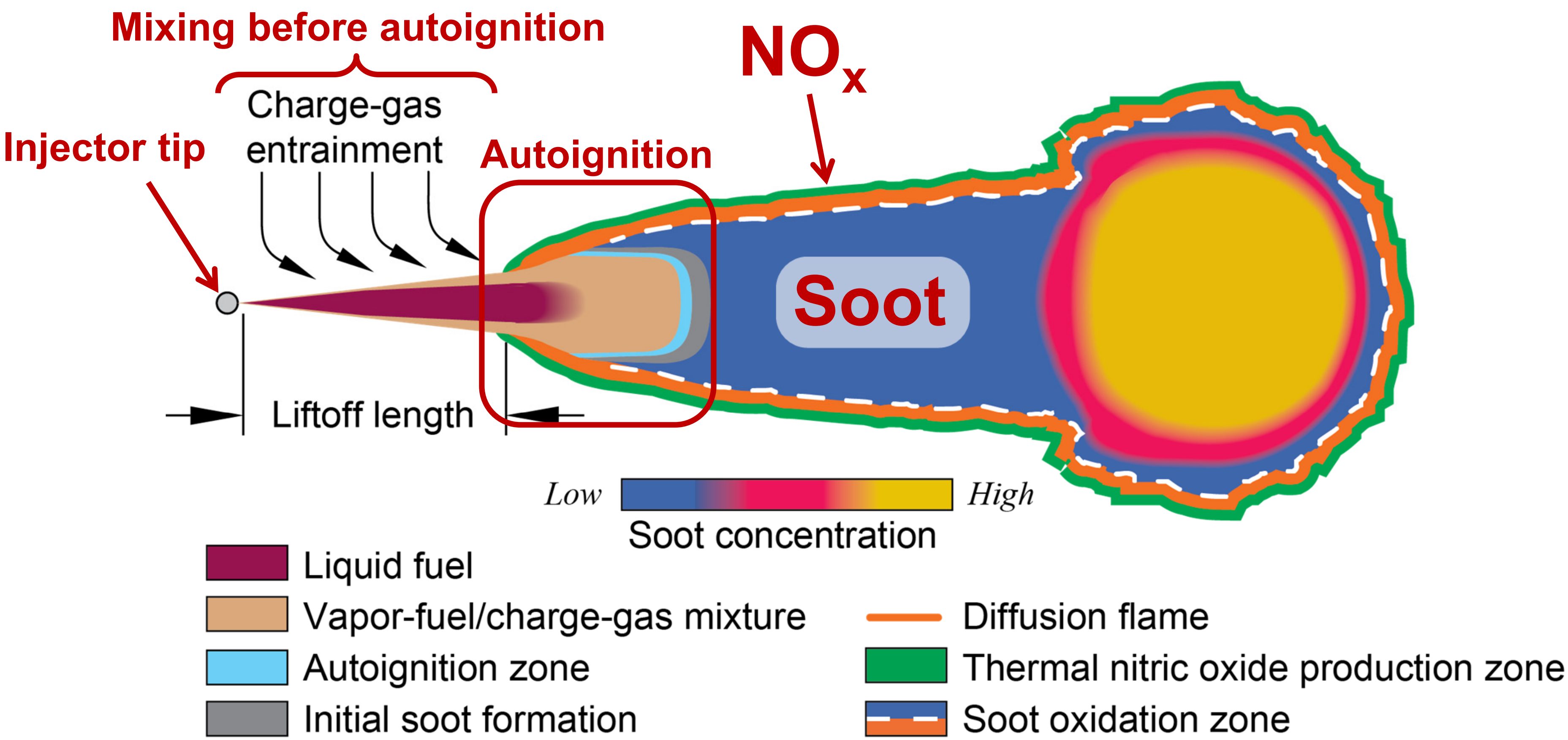
BACKGROUND Why diesel?

- Cost-effective ✓
- Inherently high efficiency ✓
- Easy to control ignition timing ✓
- Fuel-flexible ✓
- High torque & power density ✓
- Low cyclic variability ✓
- Durable & reliable ✓
- Low hydrocarbon emissions ✓
- Low carbon monoxide emissions ✓
- Low soot emissions ✗
- Low nitrogen oxides (NO_x) emissions ✗

Conventional Diesel Combustion (CDC)

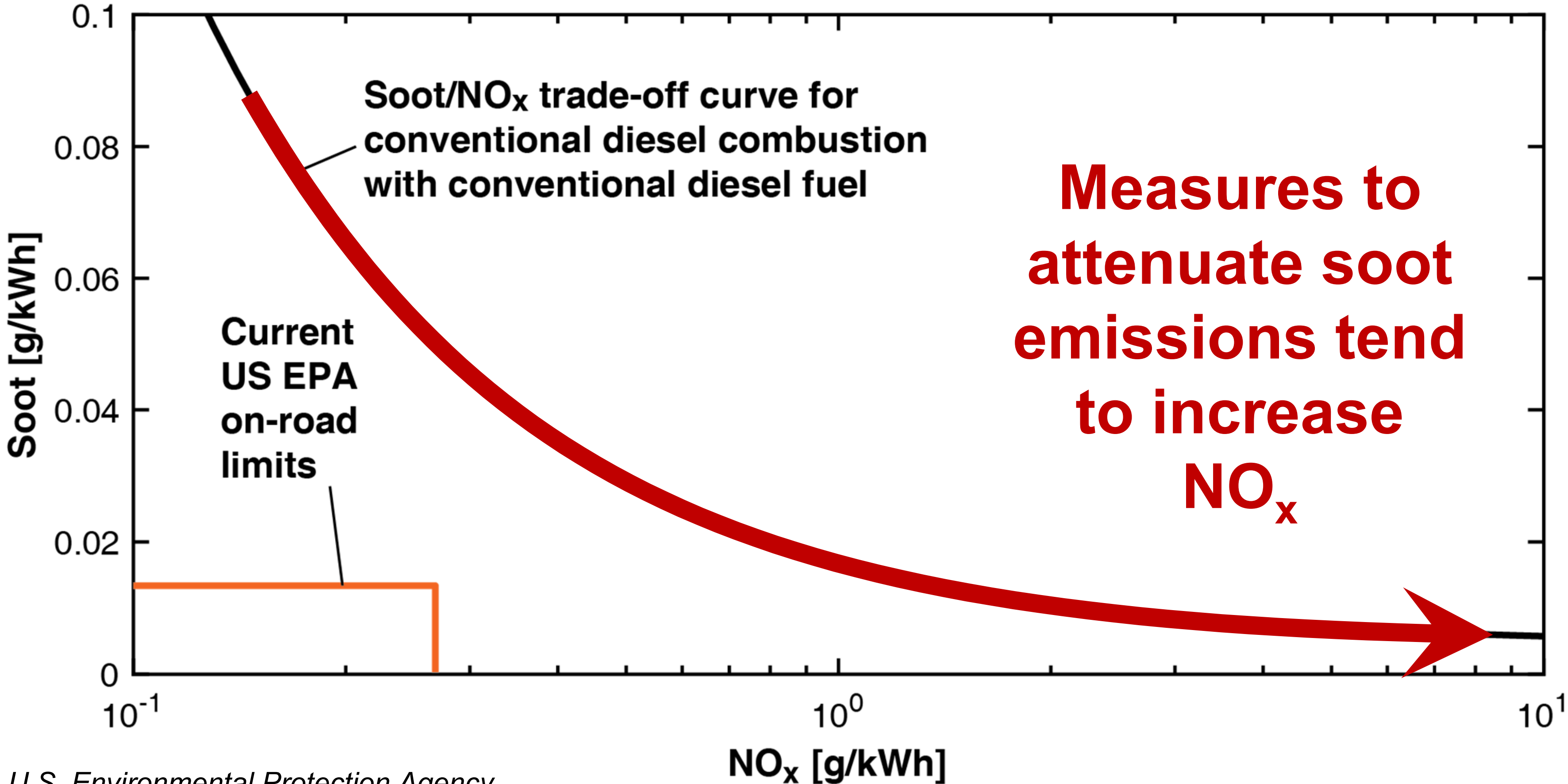


BACKGROUND Why does diesel make soot & NO_x?



Dec, J.E., doi:10.4271/970873

BACKGROUND The soot/NO_x trade-off



US EPA = U.S. Environmental Protection Agency, g = gram, kWh = kilowatt-hour

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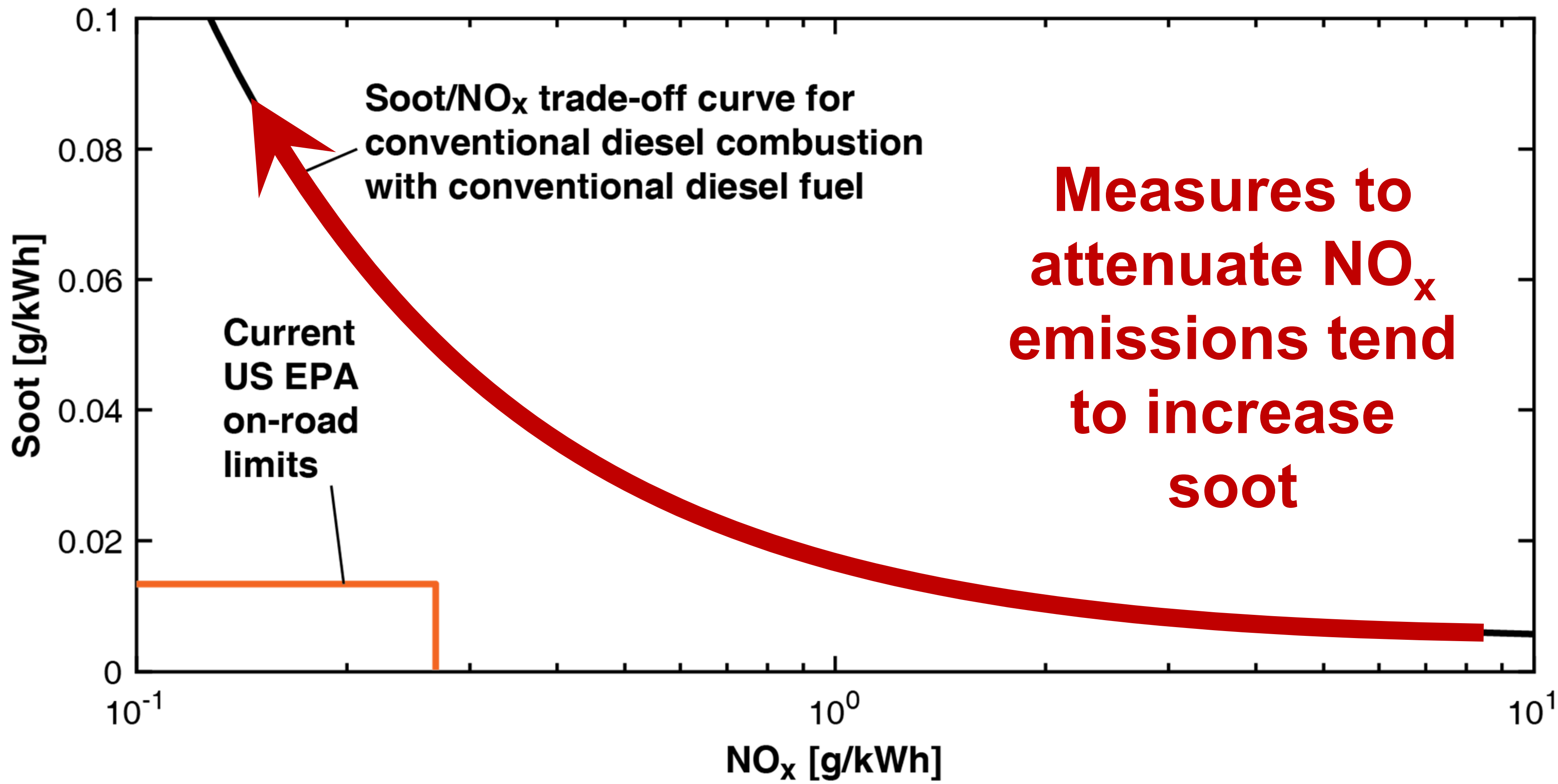

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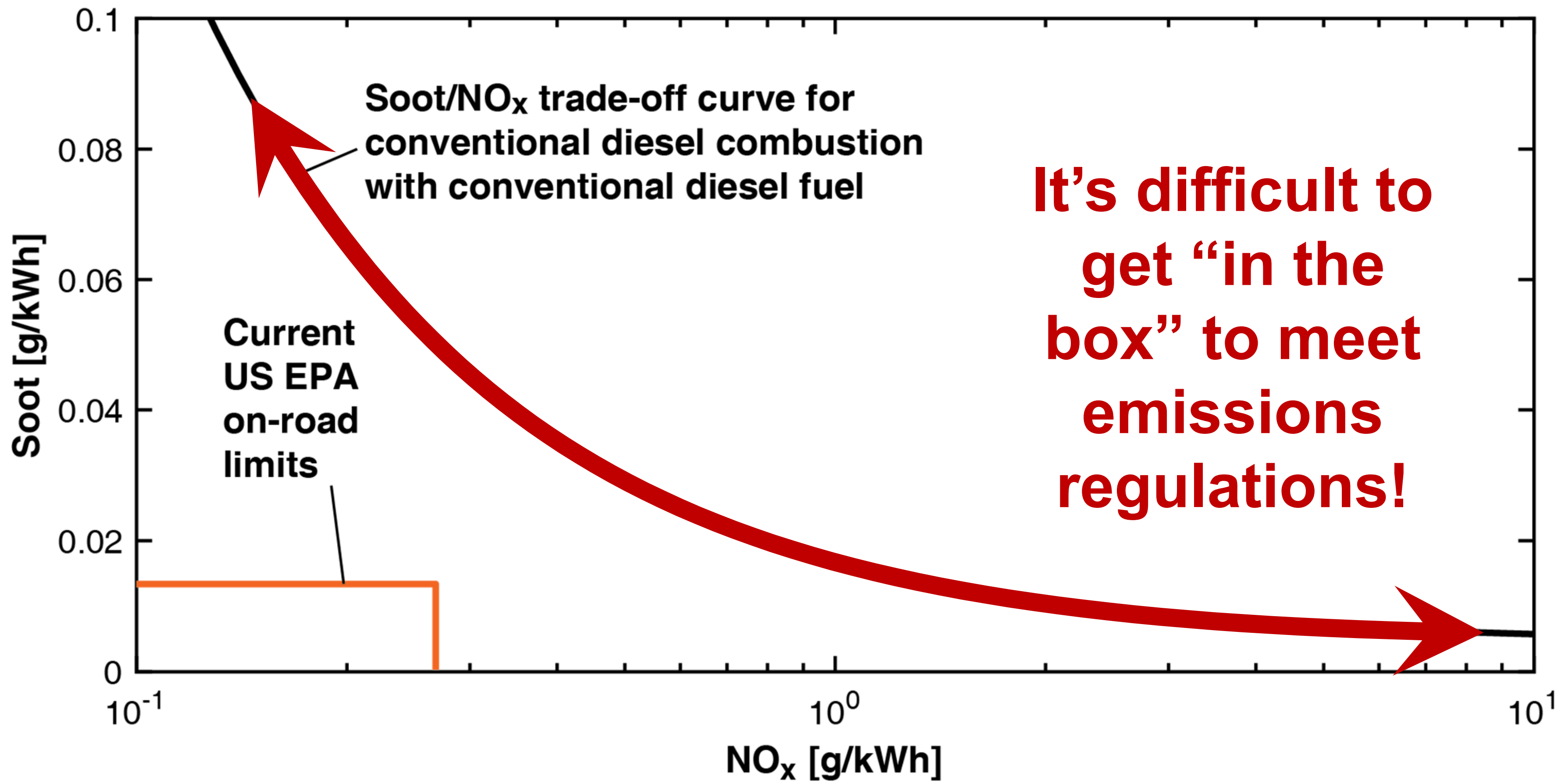
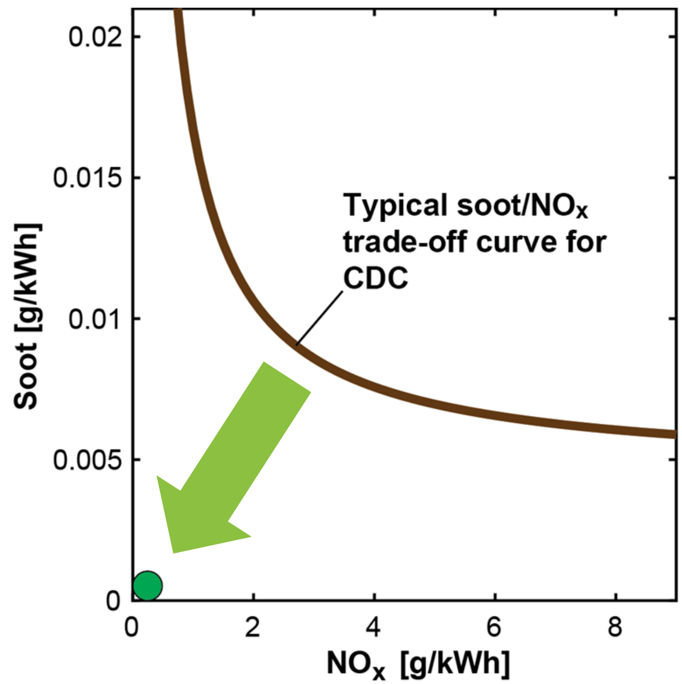


The Goal

Low-carbon fuel blendstocks and engine combustion strategies to reduce NO_x and soot emissions

OBJECTIVE Maintain all the desirable attributes of CDC…

Practical



Secure

…with 10X–100X lower soot & NO_x emissions
…while achieving net-zero carbon with home-grown fuels.

Key Takeaways

We’re well on the path to achieving the goal

TAKEAWAYS We're well on the path to achieving the goal

- Screened hundreds to thousands of potential fuels to identify those meeting critical diesel properties
- Identified those made via low-net-carbon pathways from biomass and waste feedstocks:
  - Hydrocarbons (lowest barriers to introduction)
  - Esters
  - Ethers (highest barriers to introduction)
- Ducted fuel injection with oxygenated fuel breaks the soot/NO_x trade-off
  - Maintains desirable attributes of conventional diesel combustion

Research Approach

Connect engine performance
to fuel properties to fuel chemistry

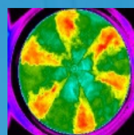
APPROACH Link properties to engine operation

Hypothesis:

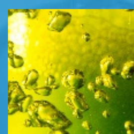
Equivalent fuel properties result in equivalent performance

- Took a fuel-properties-based, composition-agnostic approach
- Considered new engine designs for realizing emission benefits

APPROACH Link properties to engine operability and fuel handling



- Rapid fuel ignition (cetane number)



- Complete evaporation (boiling point or T90)

- Cold temperature operability (cloud point)

- Fuel pump/injector operability (viscosity)

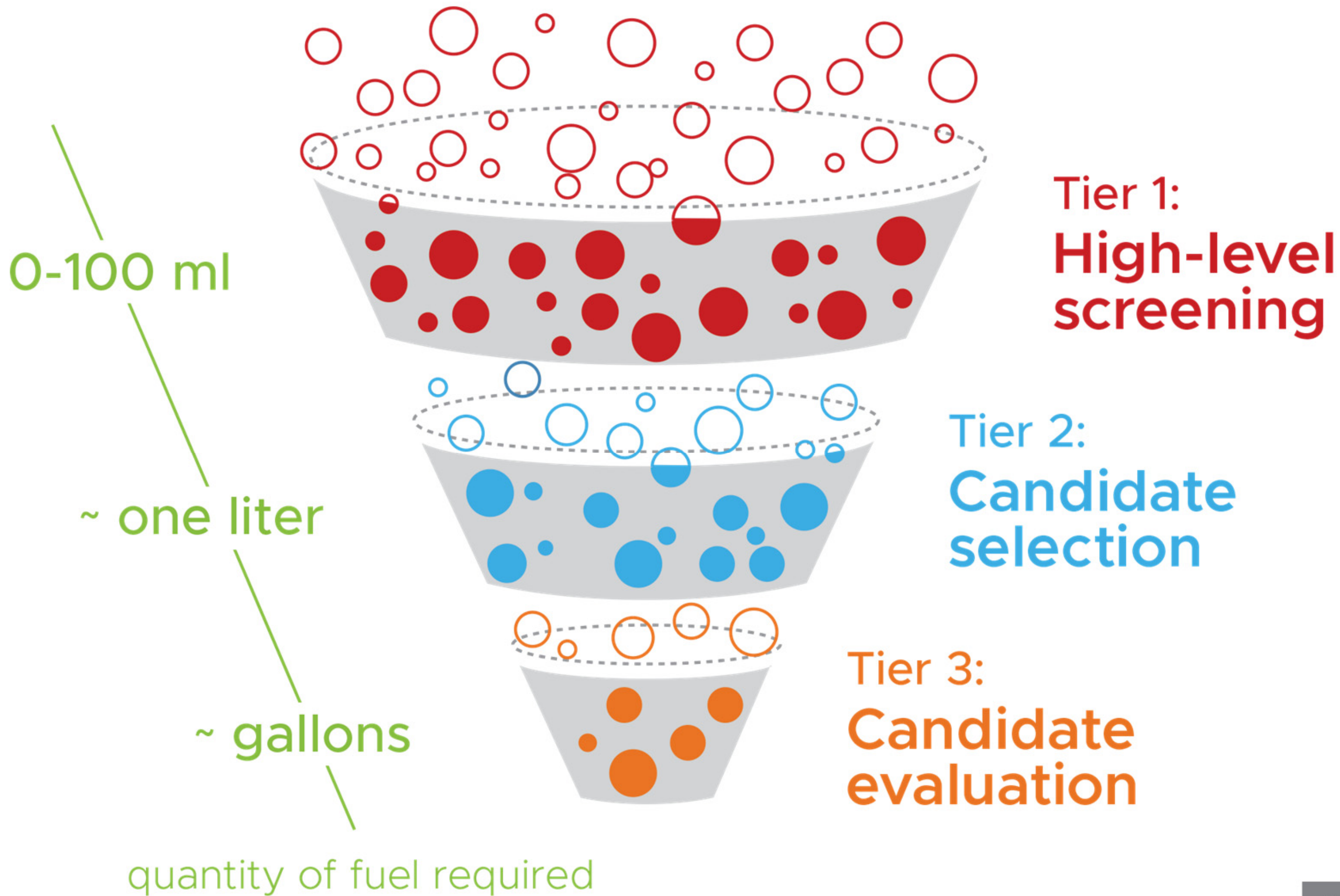
- Safety in handling (flashpoint)

- Stability in storage (oxidation stability)

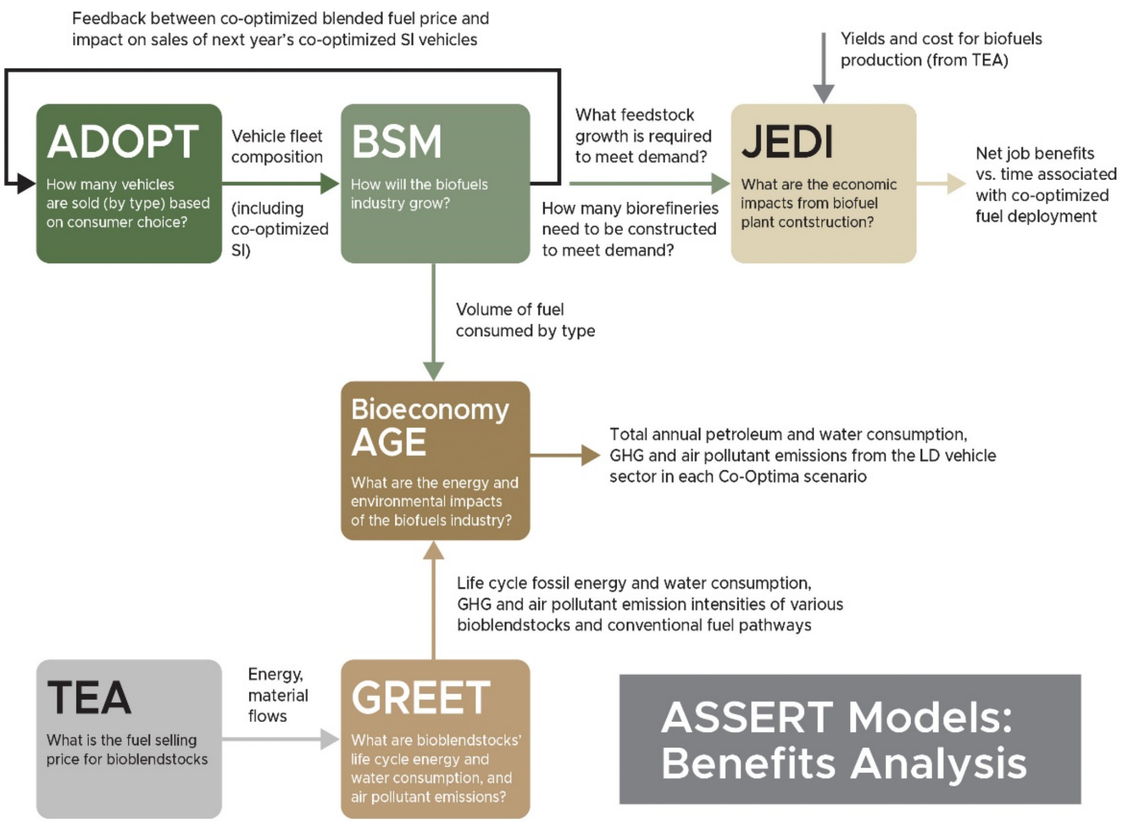
APPROACH Identify blendstocks

What biomass- and waste-derived blendstocks contribute desired fuel properties?

- Boiling point
- Flashpoint
- Melting or cloud point
- Cetane number



APPROACH Evaluate impacts



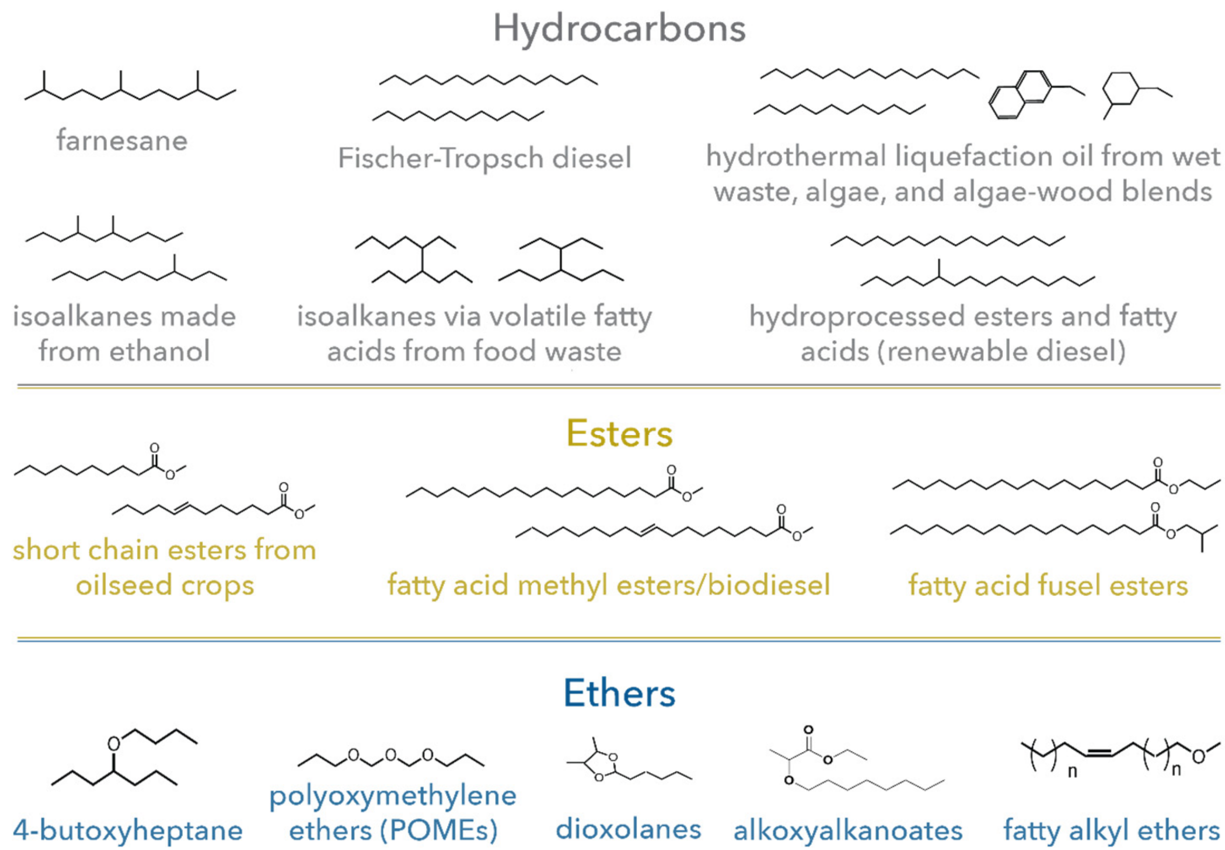
- Techno-economic and wells-to-wheels life cycle analyses inform biofuel research
- Validated models linked by analysts answer complex questions on impacts

Notable Outcomes

- Many sustainable blendstock options
- Pathway to near-zero soot and very low NO_x

OUTCOMES Many blendstock options

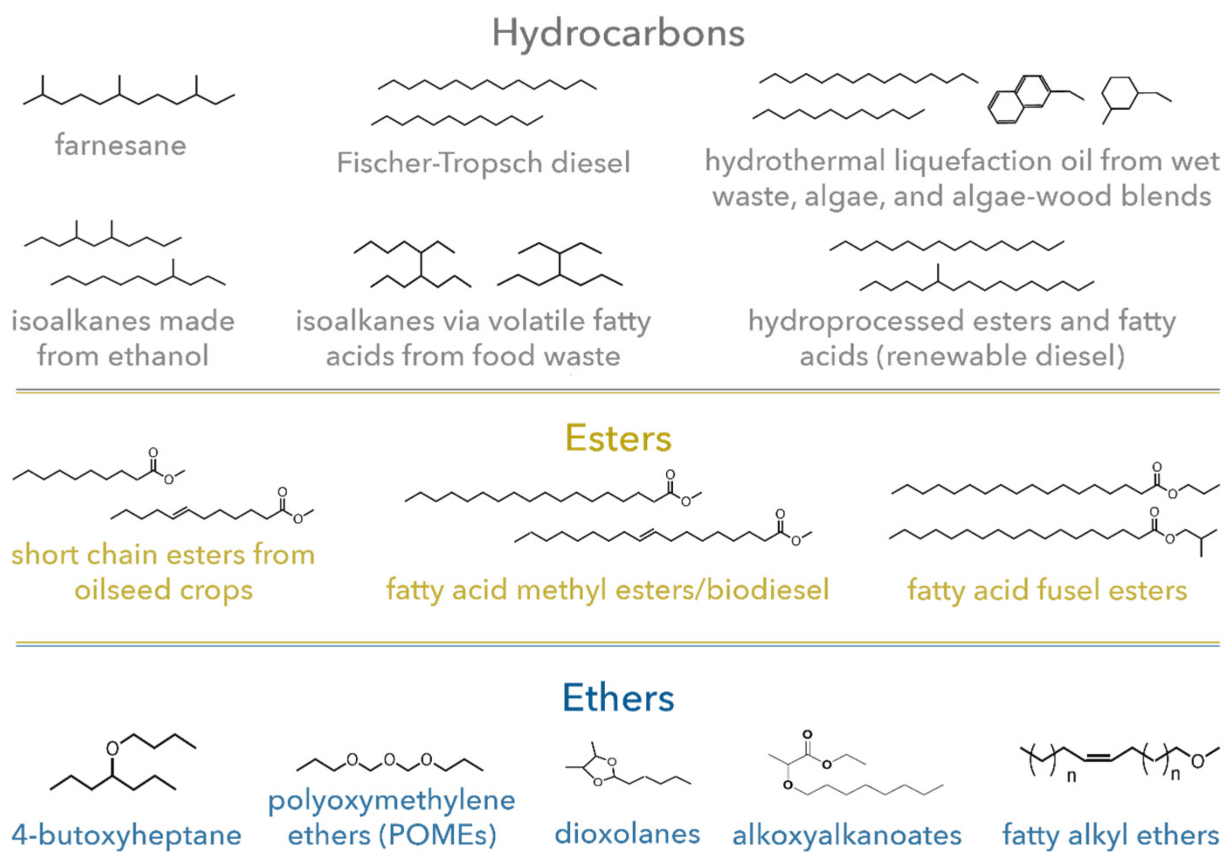
- **Cetane number > 40 (most > 48), lower heating value > 28 MJ/kg, acceptable flashpoint, cloud point, and other properties**
- **Blendstock greenhouse gas (GHG) emissions reduced by 50% or >60% in many cases**
- **Potential to be produced at $5.50/GGE or better**



Top 14 MCCI blendstocks report to be released soon

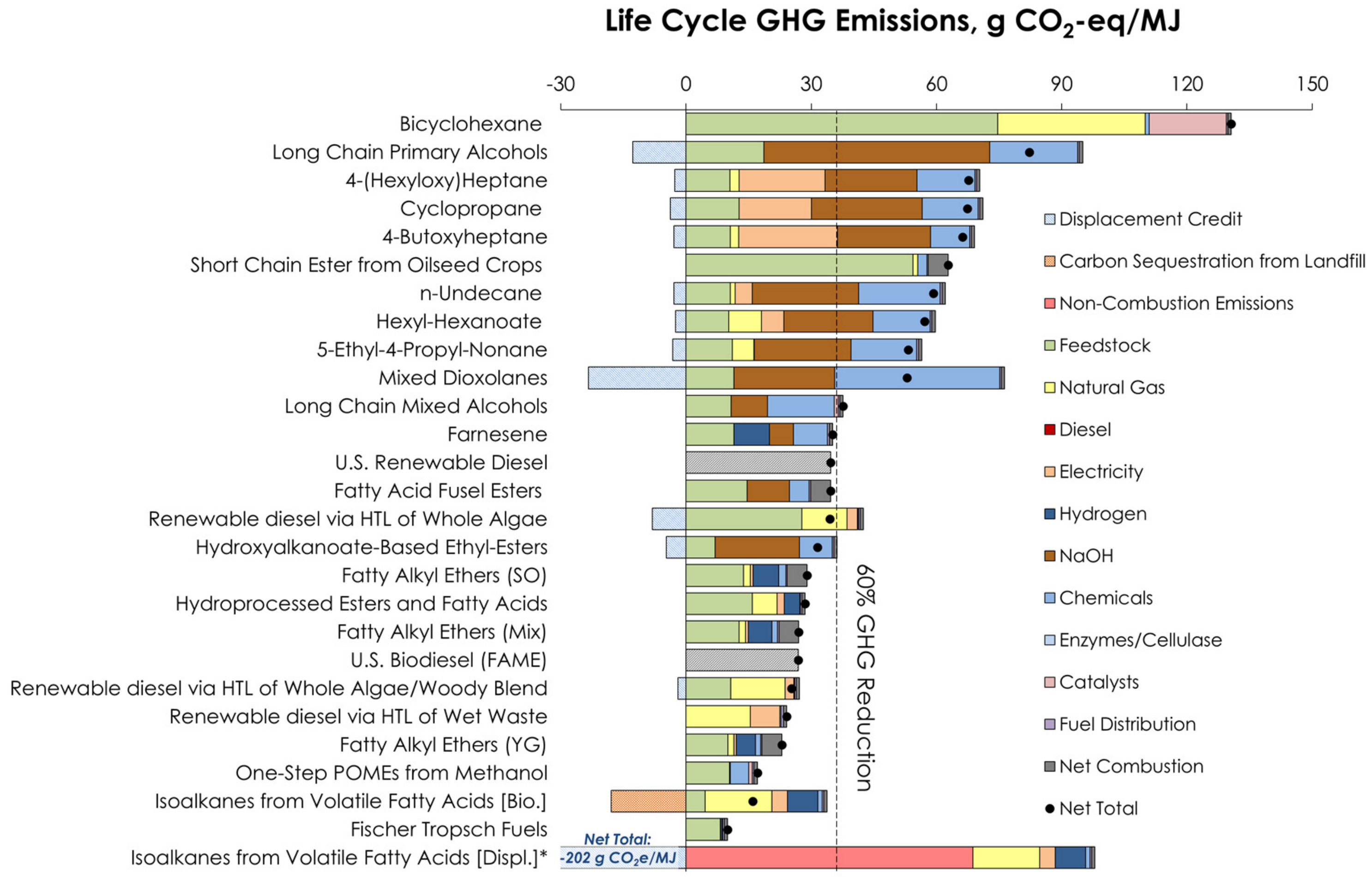
OUTCOMES Many blendstock options

- **Hydrocarbons (lowest barriers to introduction)**
  - ➢ Ester-based renewable diesel and Fischer-Tropsch diesel from natural gas are produced commercially today
- **Esters (some barriers to use at high blend levels)**
- **Ethers (highest barriers to introduction)**
  - ➢ Storage stability examined and some will require antioxidant additives
  - ➢ Assessment of toxicity and biodegradation is ongoing



OUTCOMES Biofuels reduce GHG emissions

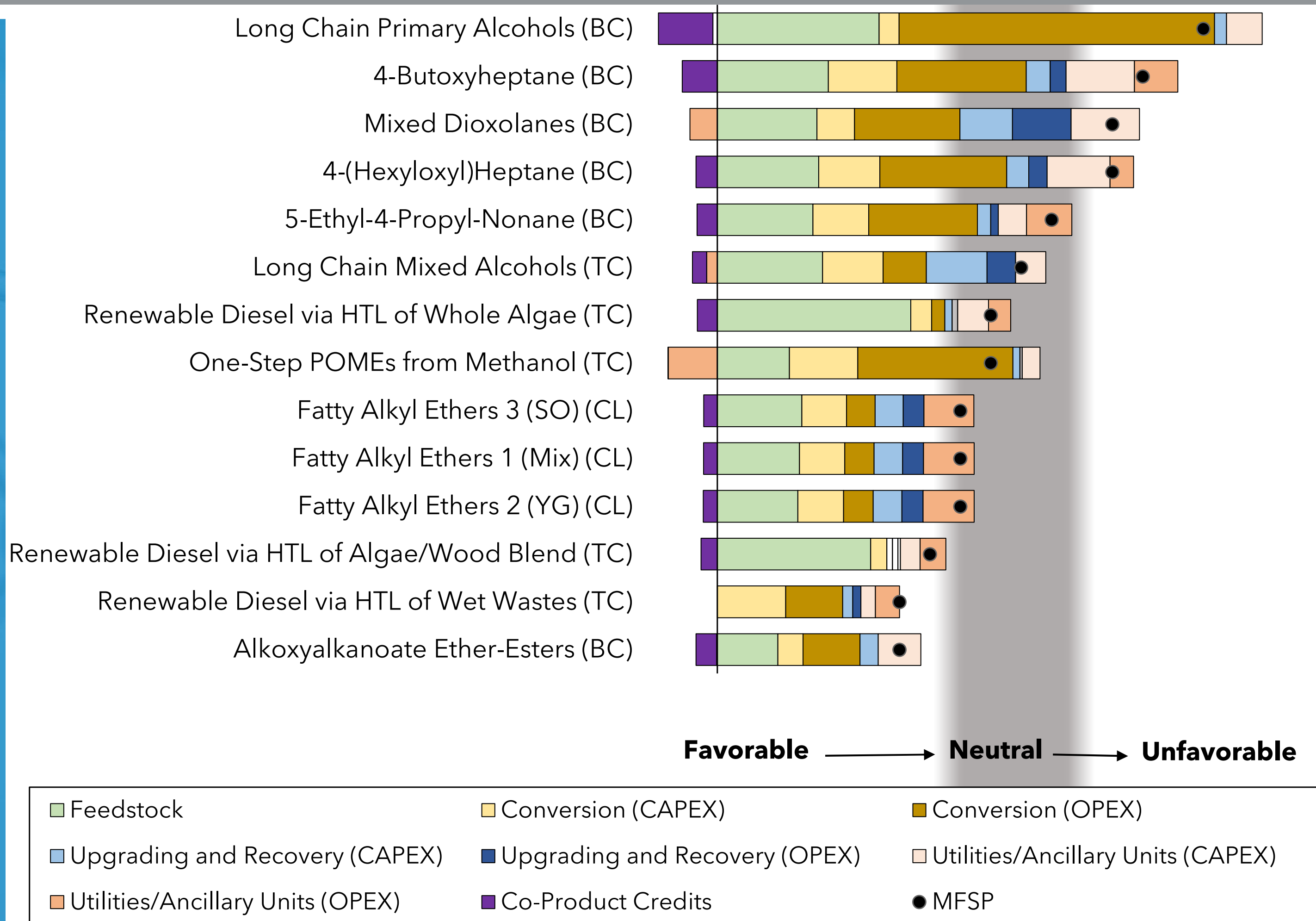
- Wide range of well-to-wheels GHG emissions reductions
- Top candidates all reduce GHG emissions by >60%
- Petroleum gasoline emissions are ~95 g CO_2 /MJ



Note: The negative GHG emissions from the "Isoalkanes from Volatile Fatty Acids" pathway is because of the credits of avoided emissions from landfill of the food waste feedstock.

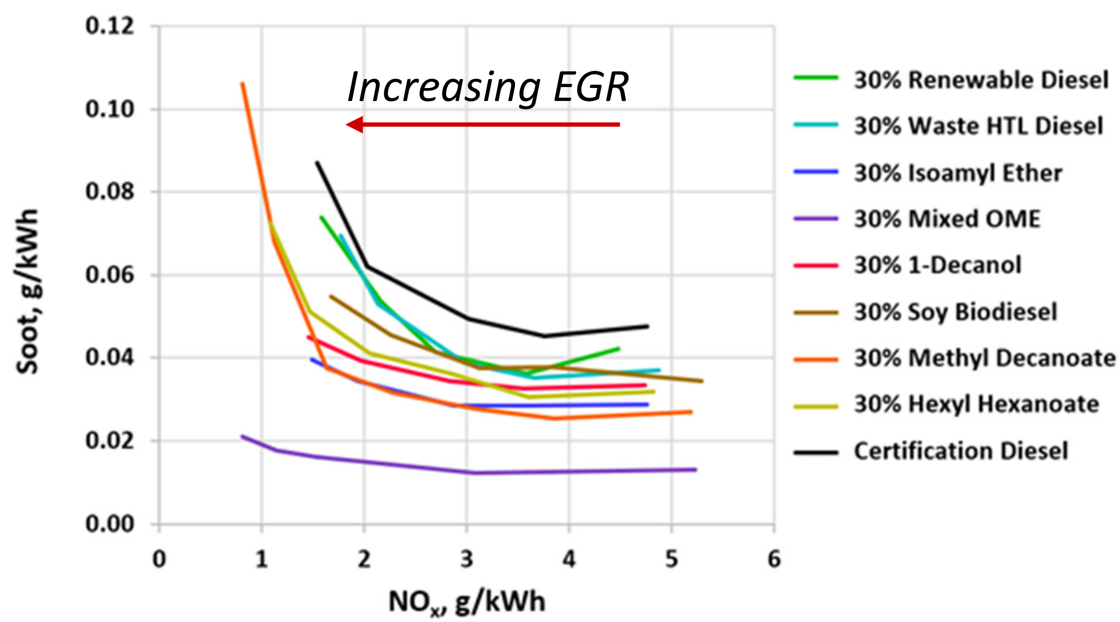
OUTCOMES Blendstocks remain more expensive than petrodiesel

- Technologies range from early R&D to pre-commercial
- Market renewable fuels (biodiesel, renewable diesel) may be constrained by feedstock supply



OUTCOMES Blendstocks reduced soot and NOx

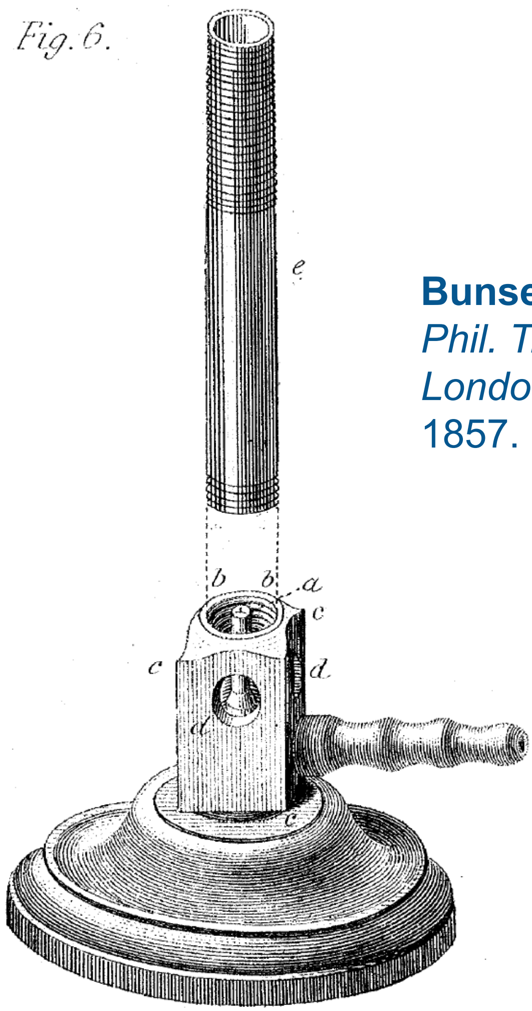
- All bioblendstocks result in lower soot
- Some blends tolerated higher levels of exhaust gas recirculation (EGR), leading to even lower NO_x



EGR tolerance = ability to maintain low soot @ high EGR

OUTCOMES Introduced ducted fuel injection (DFI)

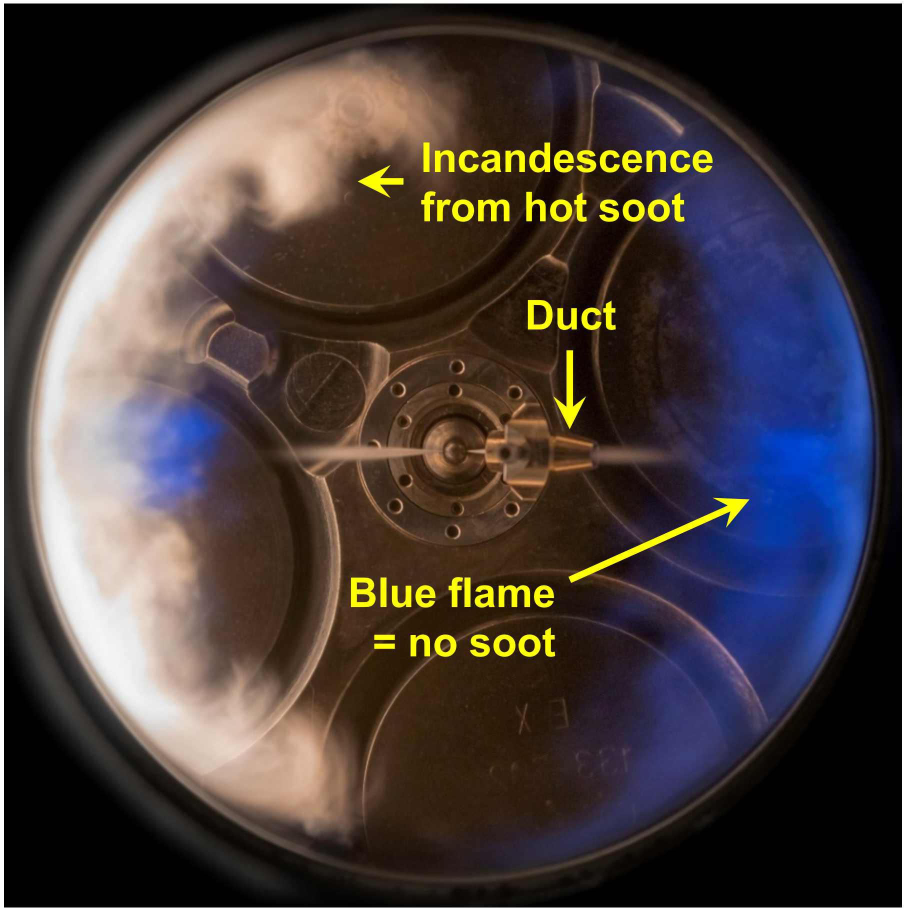
- DFI is a simple, mechanical approach for improving diesel combustion
- Motivated by the Bunsen burner concept



Bunsen and Roscoe, *Phil. Trans. Royal Soc. London* **147**:355-380, 1857.

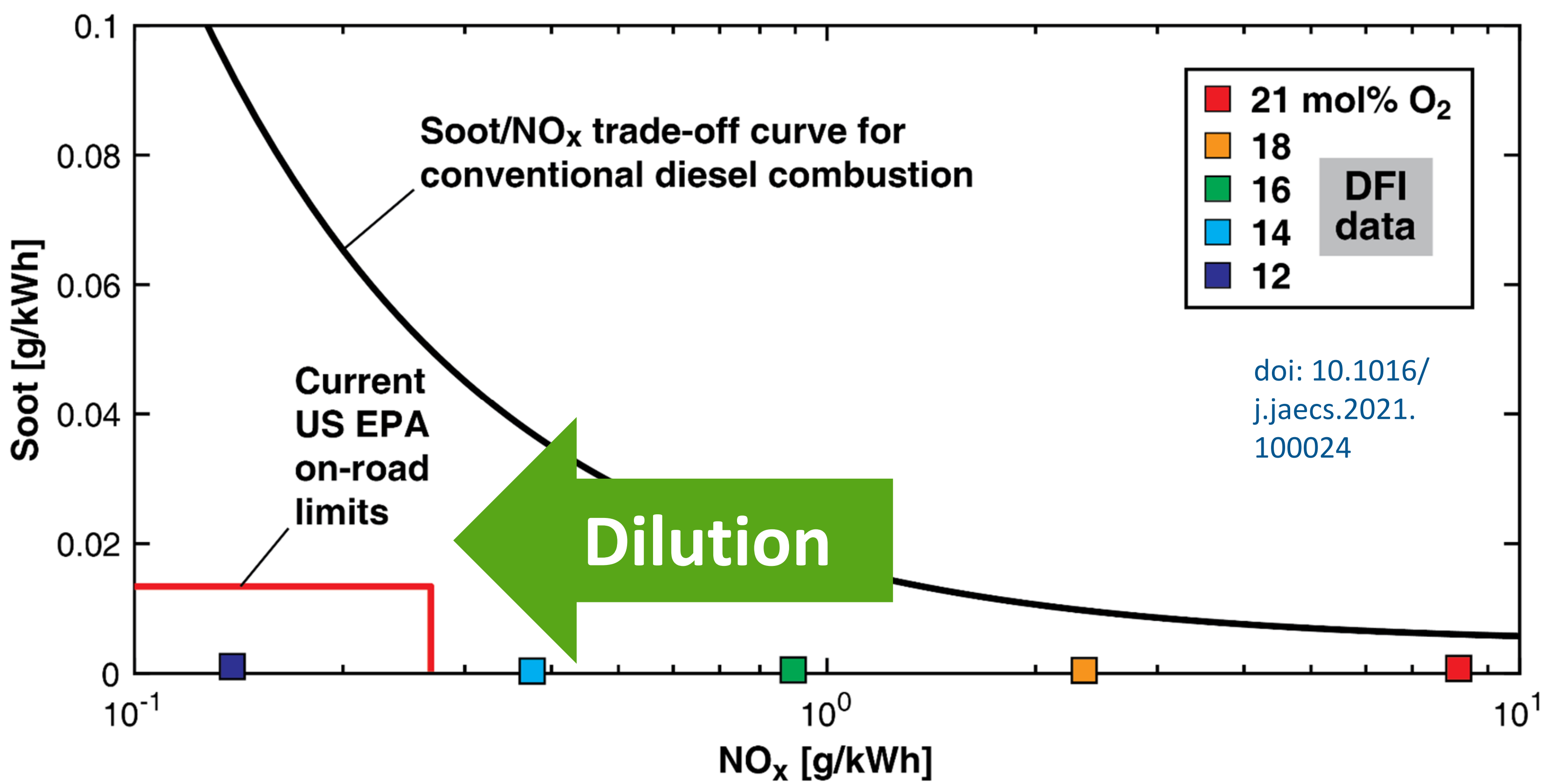
OUTCOMES First-ever engine experiments with DFI

- DFI is a simple, mechanical approach for improving diesel combustion
- Motivated by the Bunsen burner concept
- Initial engine experiments showed that DFI is effective at curtailing/ eliminating soot



S. Ashley, https://www.scientificamerican.com/article/can-diesel-finally-come-clean/

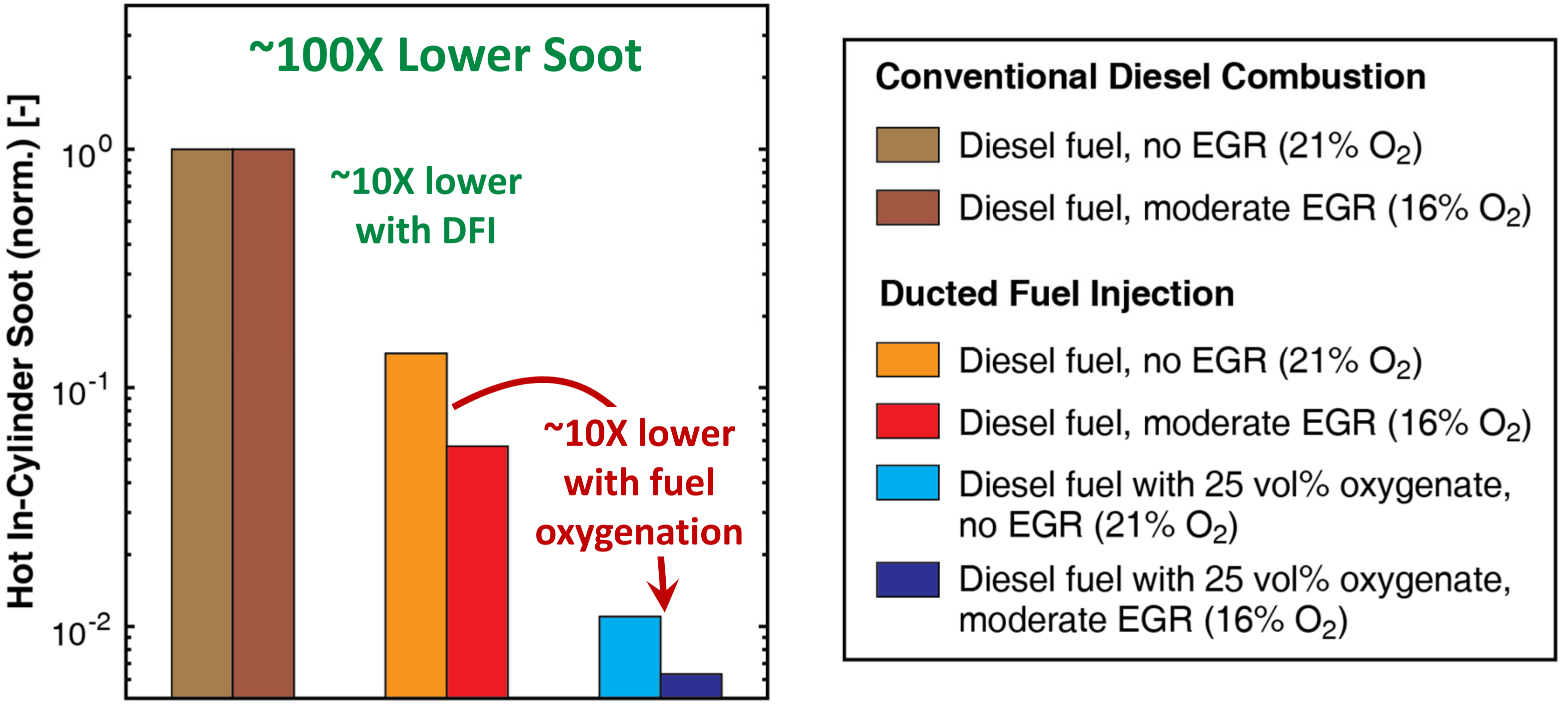
OUTCOMES DFI + dilution breaks the soot/NO_x trade-off



*Results for ~2.6 bar gross indicated mean effective pressure, 1200 rpm, steady state, 2-hole injector, No. 2 diesel fuel

OUTCOMES DFI is synergistic with oxygenated fuels

- Many low-net-CO_2, sustainable fuels are oxygenated



doi: 10.1016/j.jaecs.2021.100024

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

Next Steps

Net-zero carbon and removing barriers to market entry

Realizing the potential

- Further reduce carbon intensity
- Increase blend level
- Scaling up for commercial production while reducing GHG even further
- Learning to achieve net-zero criteria pollutants
- Overcoming 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

Acknowledgements

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Valerie Reed
Acting Director, Bioenergy Technologies Office (BETO)

Alicia Lindauer
Technology Manager, BETO Bioenergy Analysis & Sustainability

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

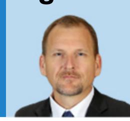
AUG 26

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?



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

Q & A

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