Co-Optima Capstone Webinar Series

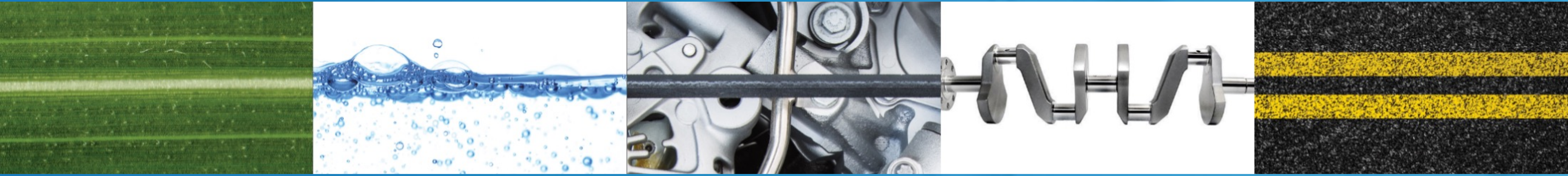
What environmental and economic benefits might be realized by co-optimizing fuels and engines for light-duty passenger vehicles?

Avantika Singh – National Renewable Energy Laboratory

May 27, 2021

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



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Overview

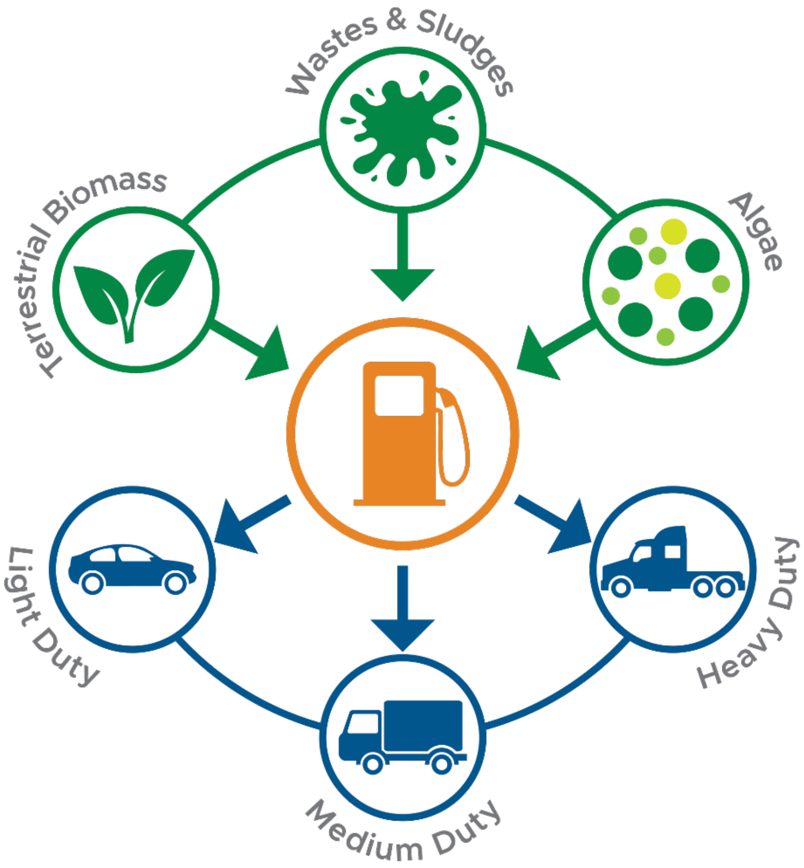
- Goal
- Key Takeaways
- Research Approach
- Notable Outcomes
- Next Steps

Better fuels. Better engines. Sooner.

Engine R&D

Fuel R&D

Seeking sustainable fuel-engine combinations



- Focus on liquid fuels
- Consider non-food-based biofuel feedstocks
- Assess well-to-wheels impacts for biofuel options
- Generate insights on value to refiners, trajectory of vehicle adoption, and socioeconomic benefits
- Provide data, tools, and knowledge

On-road transportation, light duty (LD) to heavy duty (HD)

LIGHT DUTY

- **Near term:** Turbocharged spark-ignition (SI) combustion
- **Longer term:** Multimode combustion

MEDIUM AND HEAVY DUTY

- **Near term:** Diesel combustion
- **Longer term:** Advanced compression ignition

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 and engines: past, present, and future—what did we learn and where do we go next?


Robert Wagner
Oak Ridge National Laboratory

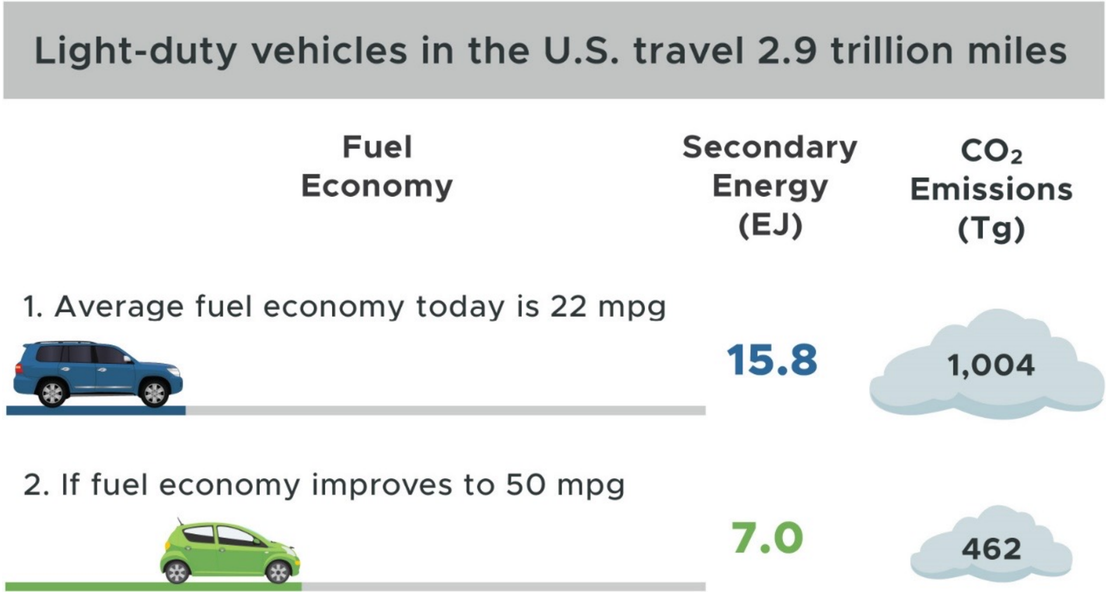

Daniel Gaspar
Pacific Northwest National Laboratory

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

Goal

Quantify economic and environmental benefits of using high-octane biofuels

GOAL Increase light-duty fleet efficiency, reduce emissions



Light-duty vehicles in the U.S. travel 2.9 trillion miles

Fuel Economy	Secondary Energy (EJ)	CO_2 Emissions (Tg)
1. Average fuel economy today is 22 mpg	15.8	1,004
2. If fuel economy improves to 50 mpg	7.0	462

Source: 2017, DOT

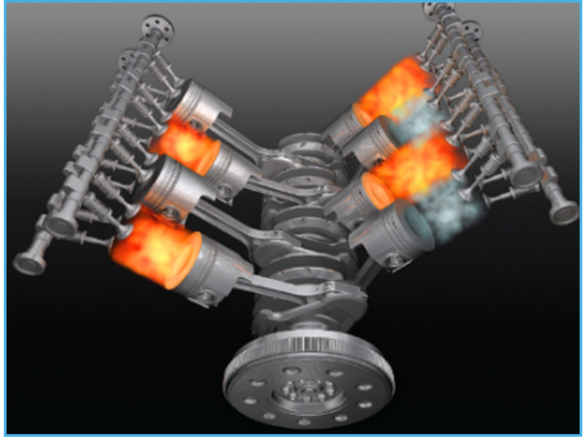
EJ = exajoule (1e18)

Tg = teragram (1e12)

- Increased efficiency lowers fuel consumption and carbon emissions
- Improved fuel properties can increase engine efficiency
- Co-optimizing fuels and engines has economic and environmental impacts

GOAL Determine cost, environmental impacts for LD sector

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

Photos courtesy of iStock

Key Takeaways

Performance advantaged, low carbon biofuels provide value to the economy

TAKEAWAYS Potential impacts in the LD sector

- Lower fuel cost per mile from higher efficiency of co-optimized vehicles
- Identified 10+ biofuels with >60% greenhouse gas (GHG) reductions vs. gasoline
- Potential value to refiners depends on
  - Blending level
  - Fuel properties: research octane number (RON) and octane sensitivity (S)
  - Refinery configuration
  - Fuel demand
- Co-optimized fuels and engines offer reductions in
  - Petroleum consumption
  - GHG emissions
  - Water consumption
  - Fine particulate matter ($PM_{2.5}$) emissions

Research Approach

Deploy integrated modeling tools to perform comprehensive analysis

APPROACH

Comprehensive benefits and risk analysis

LD Fuels and Combustion Modes

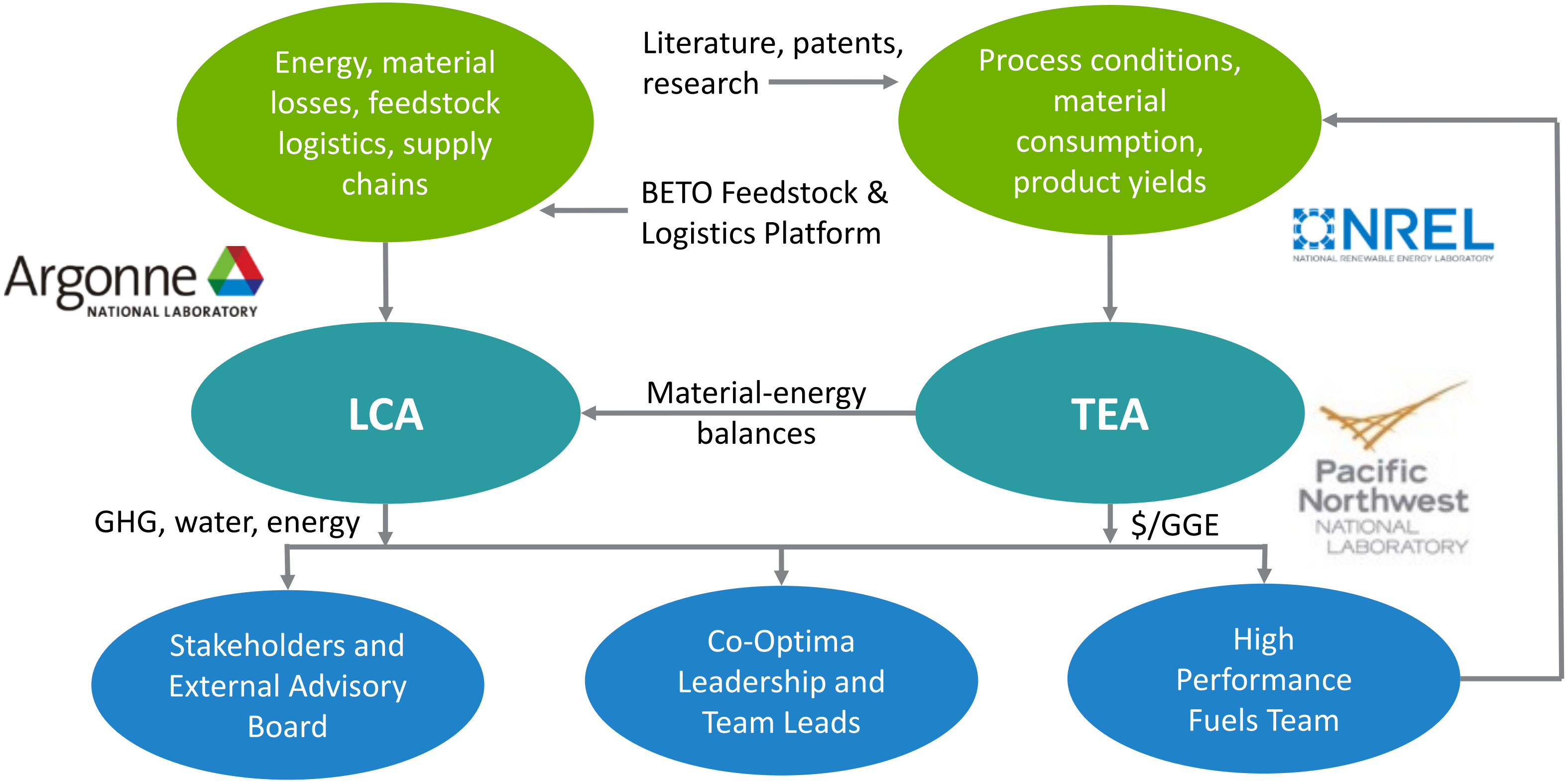
Biofuel Production
How cost-effective is it to produce Co-Optima biofuels?

Refinery Benefits
What is the value of Co-Optima biofuels to the refining industry?

Vehicle Adoption
How would Co-Optima vehicle technology penetrate the market?

Economy-wide Benefits
Any socioeconomic benefits of Co-Optima fuels/vehicle adoption?

APPROACH TEA and LCA inform research direction



Energy, material losses, feedstock logistics, supply chains

Literature, patents, research

Process conditions, material consumption, product yields

BETO Feedstock & Logistics Platform

Argonne NATIONAL LABORATORY

NREL NATIONAL RENEWABLE ENERGY LABORATORY

LCA

Material-energy balances

TEA

Pacific Northwest NATIONAL LABORATORY

GHG, water, energy

$/GGE

Stakeholders and External Advisory Board

Co-Optima Leadership and Team Leads

High Performance Fuels Team

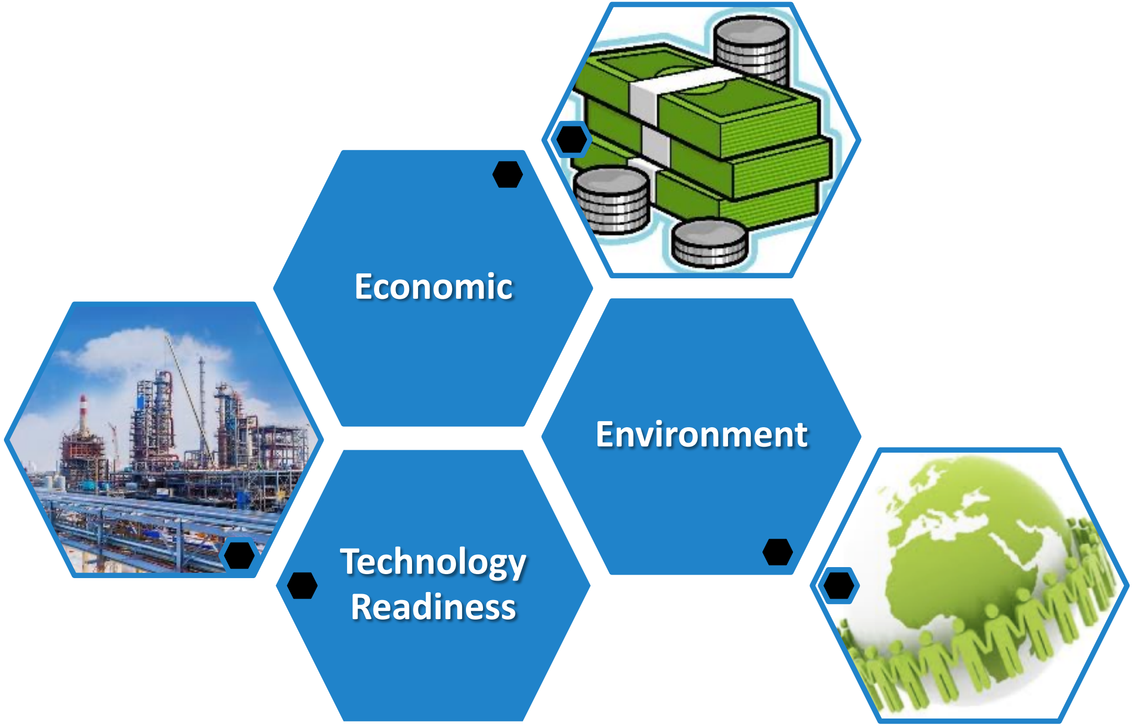
BETO = Bioenergy Technologies Office, GGE = gasoline gallon equivalent, LCA = life cycle analysis, TEA = techno-economic analysis

APPROACH Metrics to classify scale-up potential

- Economic, environmental, and scalability metrics

- Current baseline and future target cases

- 19 metrics characterized as
  - Favorable
  - Neutral
  - Unfavorable
  - Unknown



Economic

Environment

Technology Readiness

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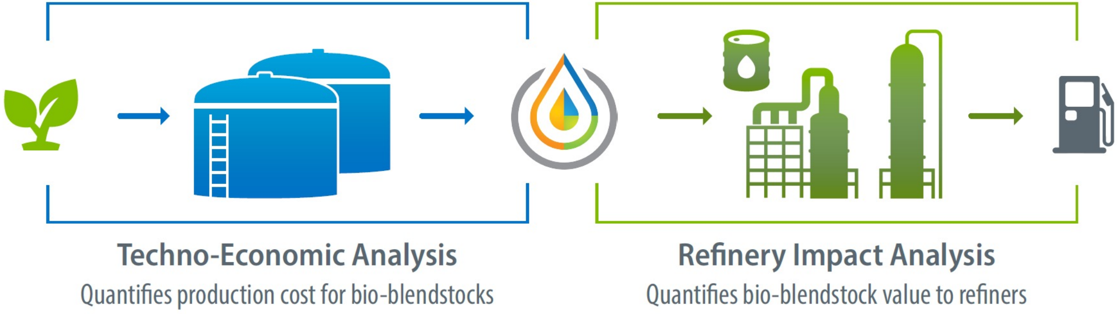
APPROACH Identify biofuel value using refinery tools



Benchmark against business-as-usual case, quantify

- refinery-wide cost of blending biofuels
- environmental performance of refinery products

- Identify fuel properties that would generate market pull from refiners
- Determine cost and sustainability implications

APPROACH Biofuel blending impacts on refinery ops.

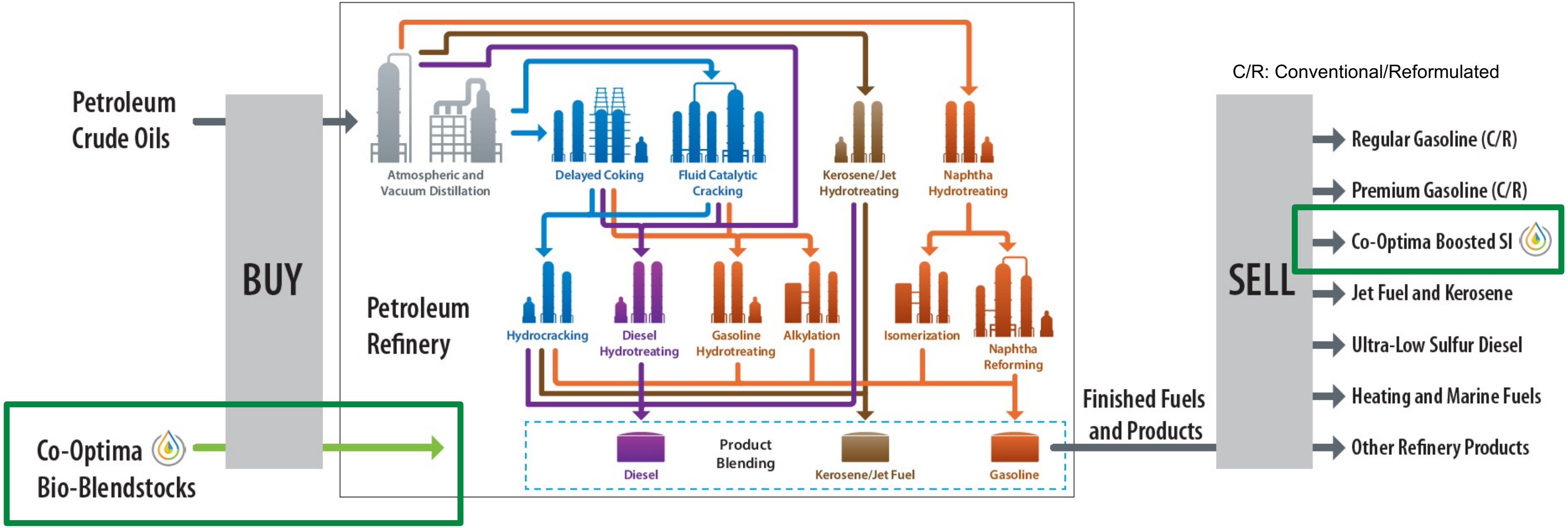
Overview of Commercial Refinery Modeling Scope in Aspen PIMS

Crude oil quality data (assays)

Pricing models for crude oils as functions of quality

Quality specifications for finished fuels

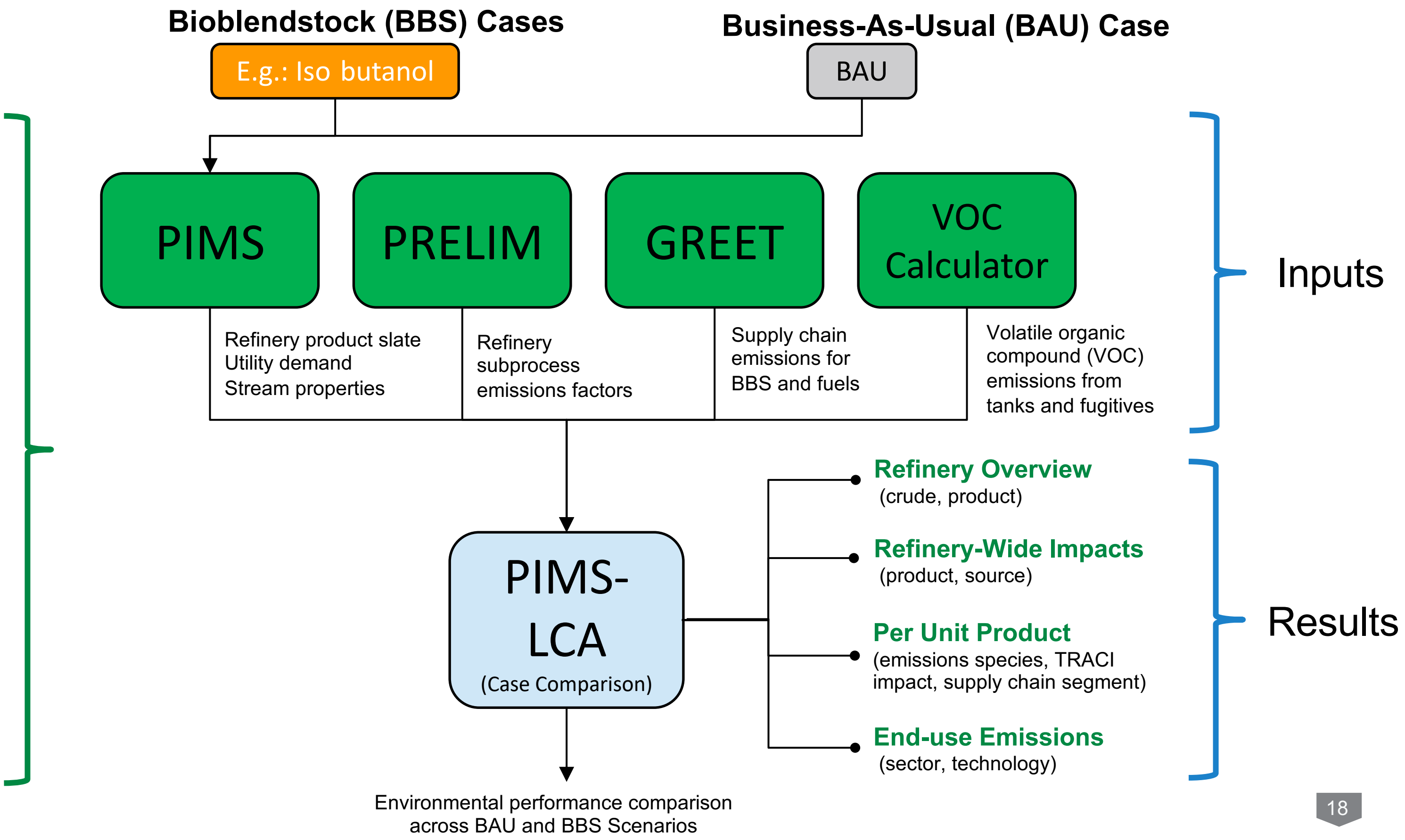
Pricing models for finished fuels and co-products



C/R: Conventional/Reformulated

APPROACH Coupled LCA to model environmental impact

Excel-based tool to inform carbon intensity of refinery emissions



Bioblendstock (BBS) Cases

E.g.: Iso butanol

Business-As-Usual (BAU) Case

BAU

PIMS

Refinery product slate
Utility demand
Stream properties

PRELIM

Refinery subprocess emissions factors

GREET

Supply chain emissions for BBS and fuels

VOC Calculator

Volatile organic compound (VOC) emissions from tanks and fugitives

Inputs

PIMS-LCA
(Case Comparison)

Refinery Overview
(crude, product)

Refinery-Wide Impacts
(product, source)

Per Unit Product
(emissions species, TRACI impact, supply chain segment)

End-use Emissions
(sector, technology)

Results

Environmental performance comparison across BAU and BBS Scenarios

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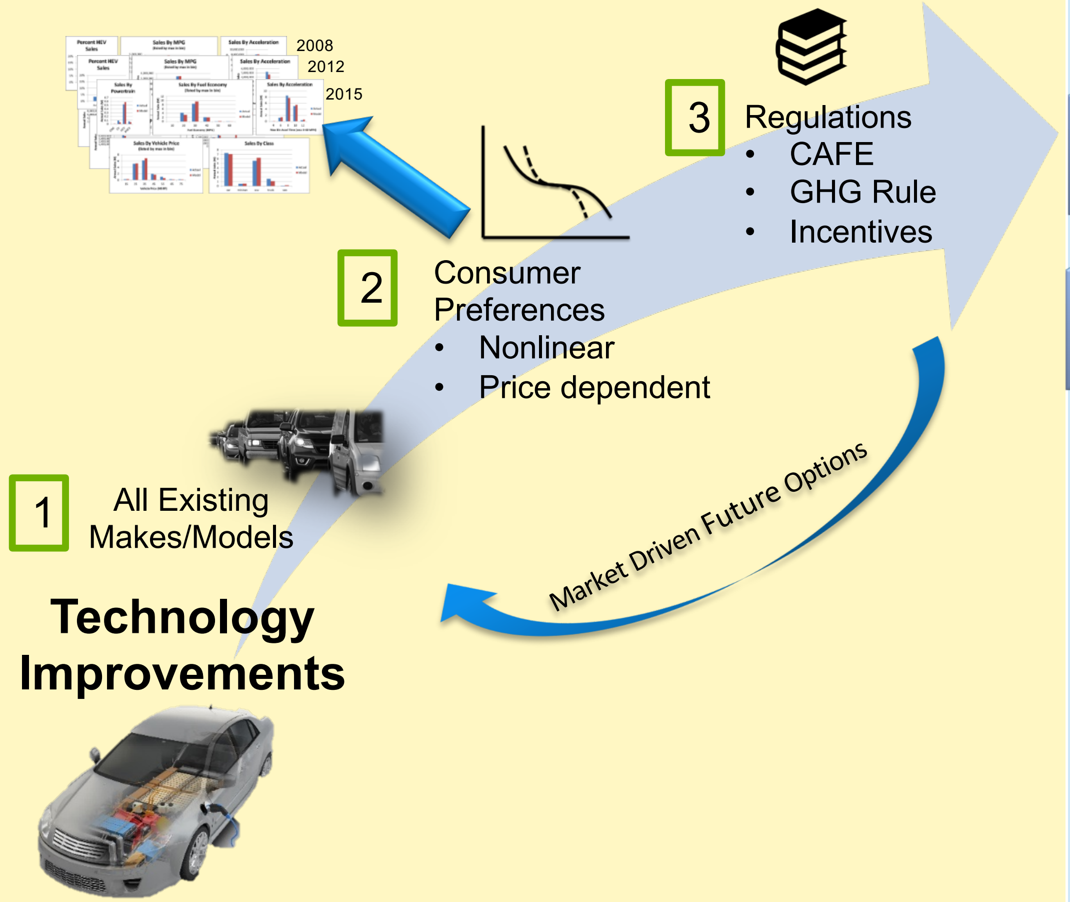
APPROACH Evolution of automobile fleet, market factors



1 All Existing Makes/Models

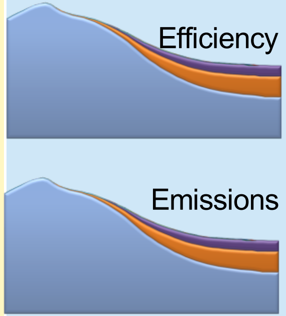
2 Consumer Preferences
- Nonlinear
- Price dependent

3 Regulations
- CAFE
- GHG Rule
- Incentives

Market Driven Future Options

Technology Improvements

Benefits



Benefits offered by Co-Optima fuels and engines

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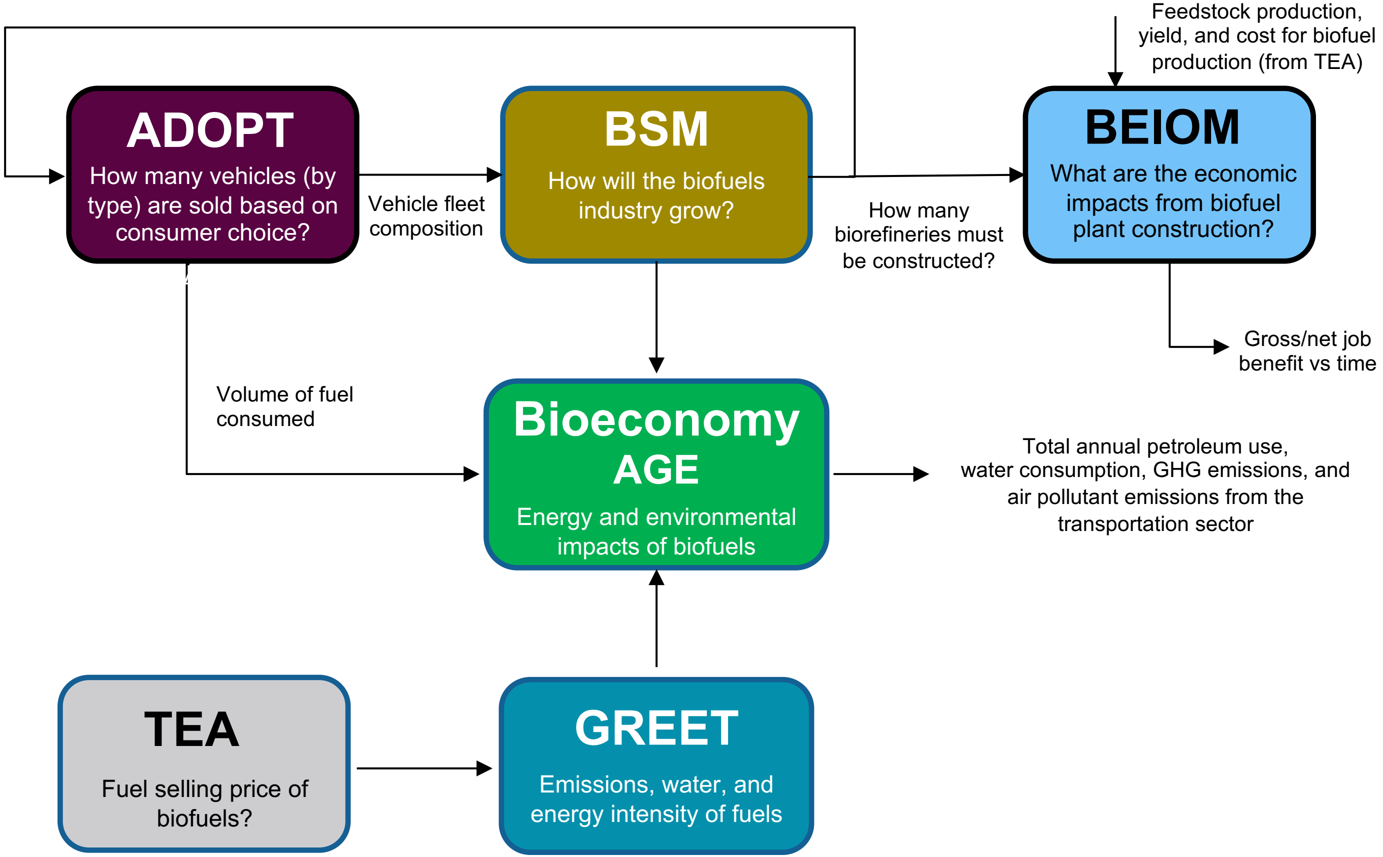
APPROACH Integrated tools evaluate cumulative benefits



Feedstock production, yield, and cost for biofuel production (from TEA)

ADOPT

How many vehicles (by type) are sold based on consumer choice?

Vehicle fleet composition

BSM

How will the biofuels industry grow?

How many biorefineries must be constructed?

BEIOM

What are the economic impacts from biofuel plant construction?

Gross/net job benefit vs time

Volume of fuel consumed

Bioeconomy AGE

Energy and environmental impacts of biofuels

Total annual petroleum use, water consumption, GHG emissions, and air pollutant emissions from the transportation sector

TEA

Fuel selling price of biofuels?

GREET

Emissions, water, and energy intensity of fuels

Notable Outcomes

Identified promising, performance-enhancing biofuels that reduce GHG emissions, improve air quality, and spur domestic job growth

OUTCOMES Comprehensive benefits and risk analysis

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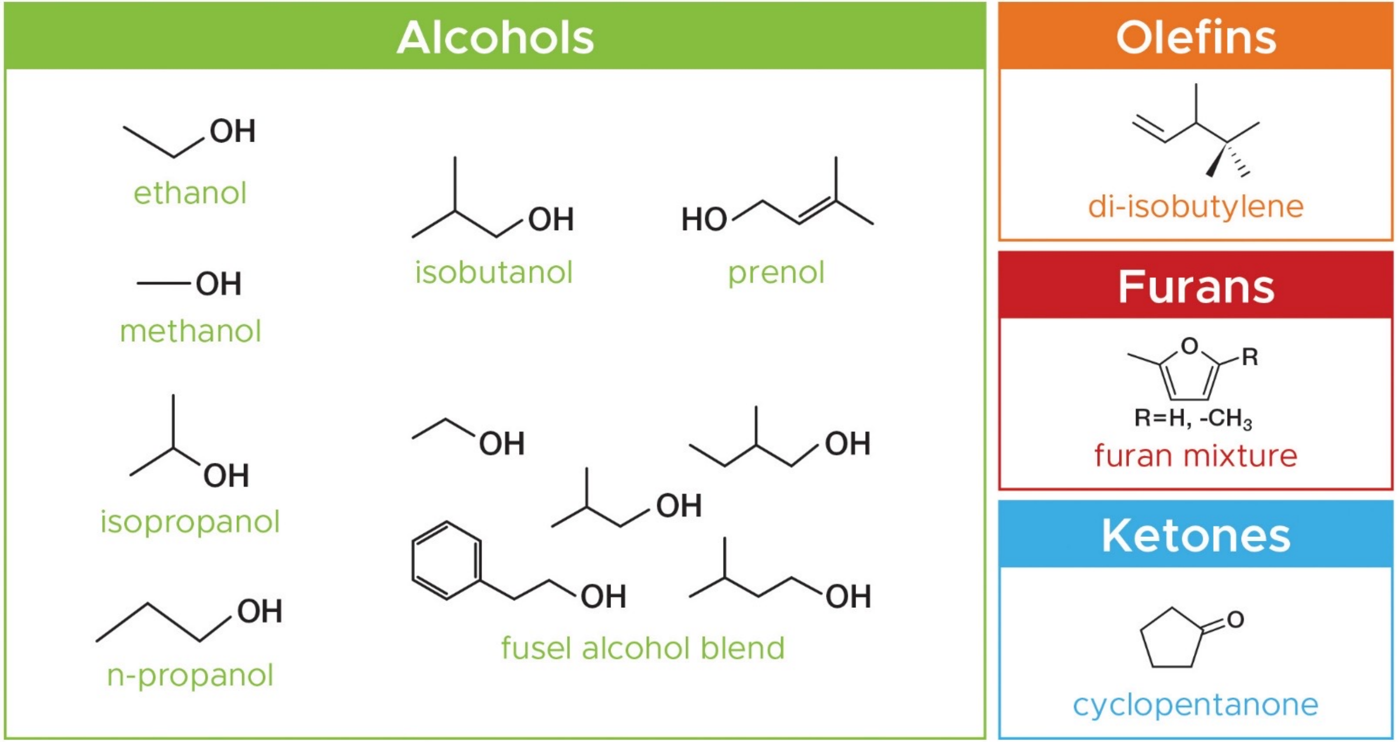
OUTCOMES Many blendstock options identified

- All have high RON, S
- Smaller alcohols also have high heat of vaporization (HOV)
- Synergistic blending of RON



Top 10 Bioblendstocks for Boosted SI Report: https://www.osti.gov/servlets/purl/1567705

OUTCOMES Biofuels with potential to scale

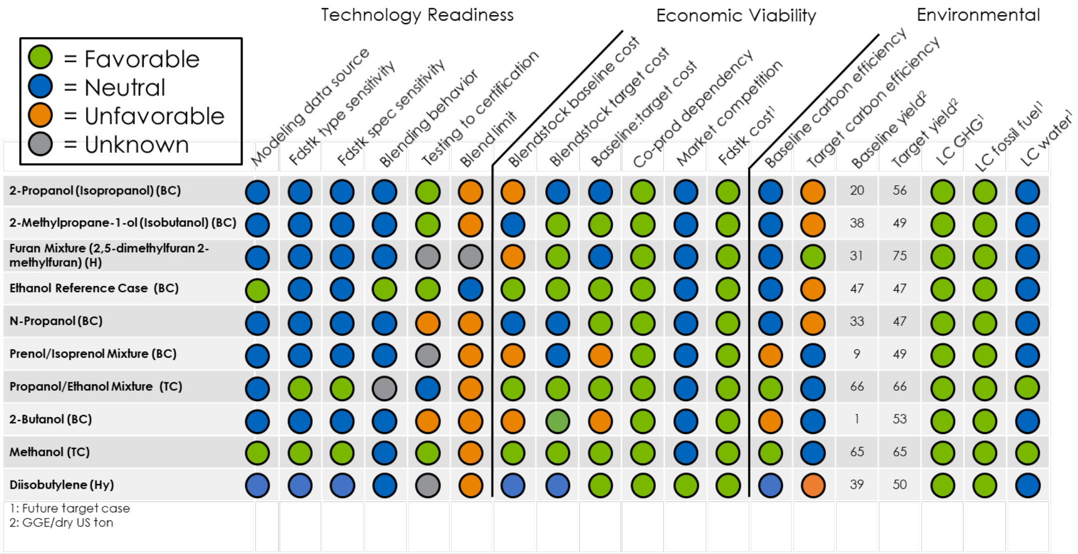
Combination of biochemical and thermochemical conversion routes

Technology Readiness

- Feedstocks available at reasonable costs and quantity
- Oxygen limits blend levels for alcohols

Economic Viability

- Many with minimum fuel selling price (MFSP) of <$4/GGE



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

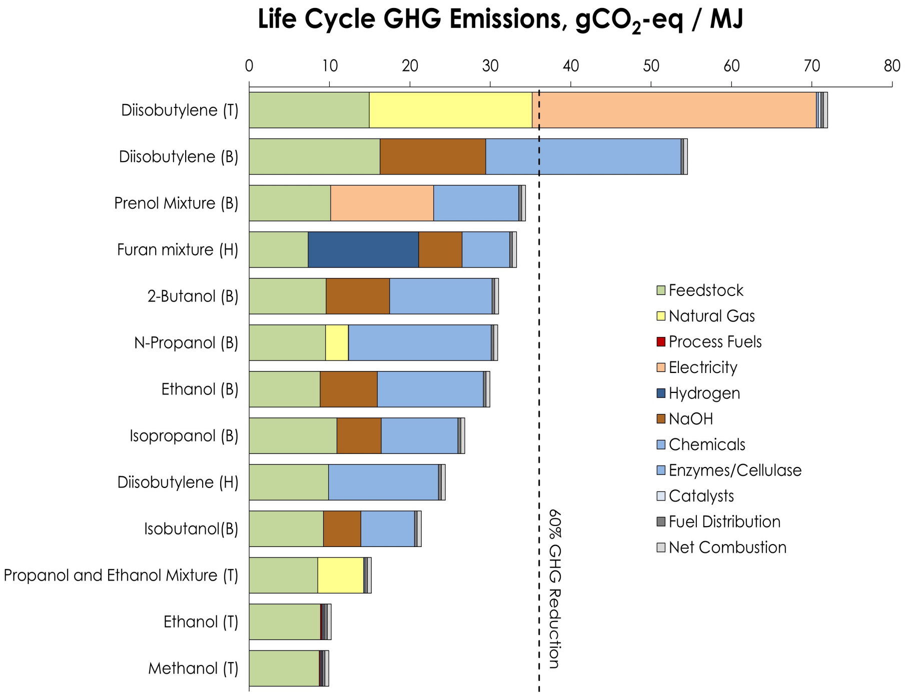
	Technology Readiness						Economic Viability						Environmental						
	Modeling data source	Fdstk type sensitivity	Fdstk spec sensitivity	Blending behavior	Testing to certification	Blend limit	Blendstock baseline cost	Blendstock target cost	Baseline:target cost	Co-prod dependency	Market competition	Fdstk cost^{1}	Baseline carbon efficiency	Target carbon efficiency	Baseline yield^{2}	Target yield^{2}	LC GHG^{1}	LC fossil fuel^{1}	LC water^{1}
2-Propanol (Isopropanol) (BC)	🔵	🔵	🔵	🔵	🟢	🟠	🟠	🔵	🔵	🟢	🔵	🟢	🔵	🟠	20	56	🟢	🟢	🔵
2-Methylpropane-1-ol (Isobutanol) (BC)	🔵	🔵	🔵	🔵	🟢	🟠	🔵	🟢	🟢	🟢	🔵	🟢	🔵	🟠	38	49	🟢	🟢	🔵
Furan Mixture (2,5-dimethylfuran 2-methylfuran) (H)	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🟢	🔵	🟢	🔵	🟢	🔵	🟢	31	75	🟢	🟢	🔵
Ethanol Reference Case (BC)	🟢	🔵	🔵	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🔵	🟢	🔵	🟠	47	47	🟢	🟢	🔵
N-Propanol (BC)	🔵	🔵	🔵	🔵	🟠	🟠	🔵	🔵	🟢	🟢	🔵	🟢	🔵	🟠	33	47	🟢	🟢	🔵
Prenol/Isoprenol Mixture (BC)	🔵	🔵	🔵	🔵	⚪	🟠	🟠	🔵	🟠	🟢	🔵	🟢	🟠	🔵	9	49	🟢	🟢	🔵
Propanol/Ethanol Mixture (TC)	🔵	🟢	🟢	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🔵	66	66	🟢	🟢	🟢
2-Butanol (BC)	🔵	🔵	🔵	🔵	🟠	🟠	🟠	🟢	🟠	🟢	🔵	🟢	🟠	🔵	1	53	🟢	🟢	🔵
Methanol (TC)	🟢	🟢	🟢	🔵	🟢	🟠	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🔵	65	65	🟢	🟢	🟢
Diisobutylene (Hy)	🔵	🔵	🔵	🔵	⚪	🟠	🔵	🔵	🟢	🟢	🟢	🟢	🔵	🟠	39	50	🟢	🟢	🔵

1: Future target case
2: GGE/dry US ton

Benavides, Bartling, Phillips, et al. (2021) in prep.

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 ~90 gCO_2 / MJ



Benavides, Bartling, Phillips, et al. (2021) in prep.

OUTCOMES Comprehensive benefits and risk analysis

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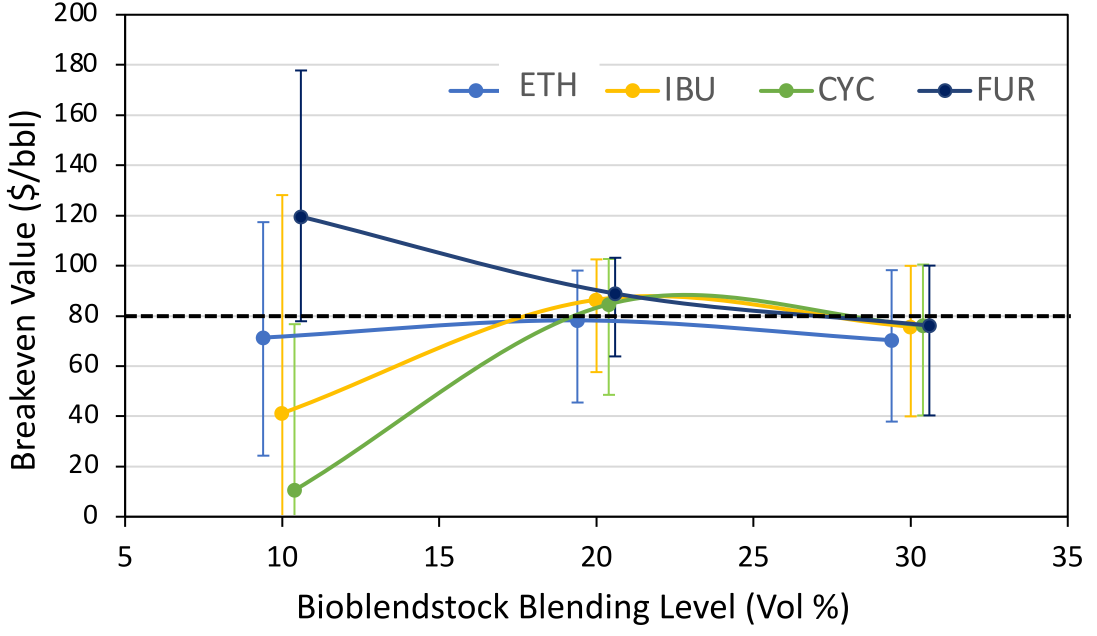
OUTCOMES RON and S drive economic benefits



ETH= ethanol; IBU=i-butanol; CYC=cyclopentanone; FUR=furans mix

(average spot price of **starch ethanol** shown by dotted line)

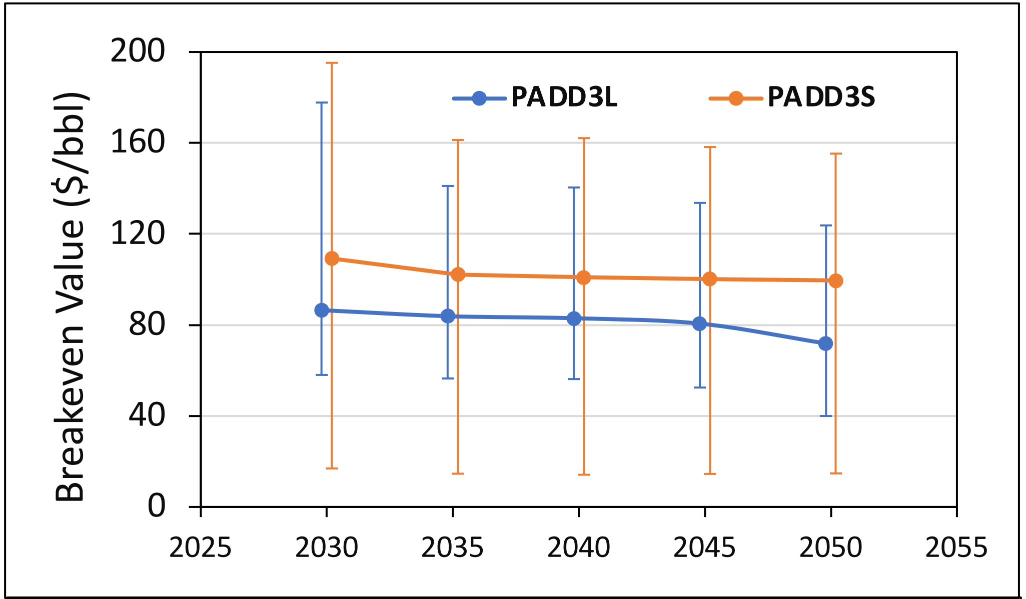
Jiang, Philips, et al. (2021) Fuel; Carlson, Singh, Talmadge, et al. (2021) in prep.

Potential value of biofuel to refiners

- Depends on fuel properties, esp. RON and S
- Varies with biofuel blending levels

Breakeven value (refinery's willingness to pay for biofuel) ranges widely from $10-120/bbl.

OUTCOMES Smaller, less complex refineries benefit more



PADD 3: Petroleum Administration for Defense Districts (Gulf Coast region)
3L: high-complexity Gulf Coast refinery; 3S: small Gulf Coast refinery

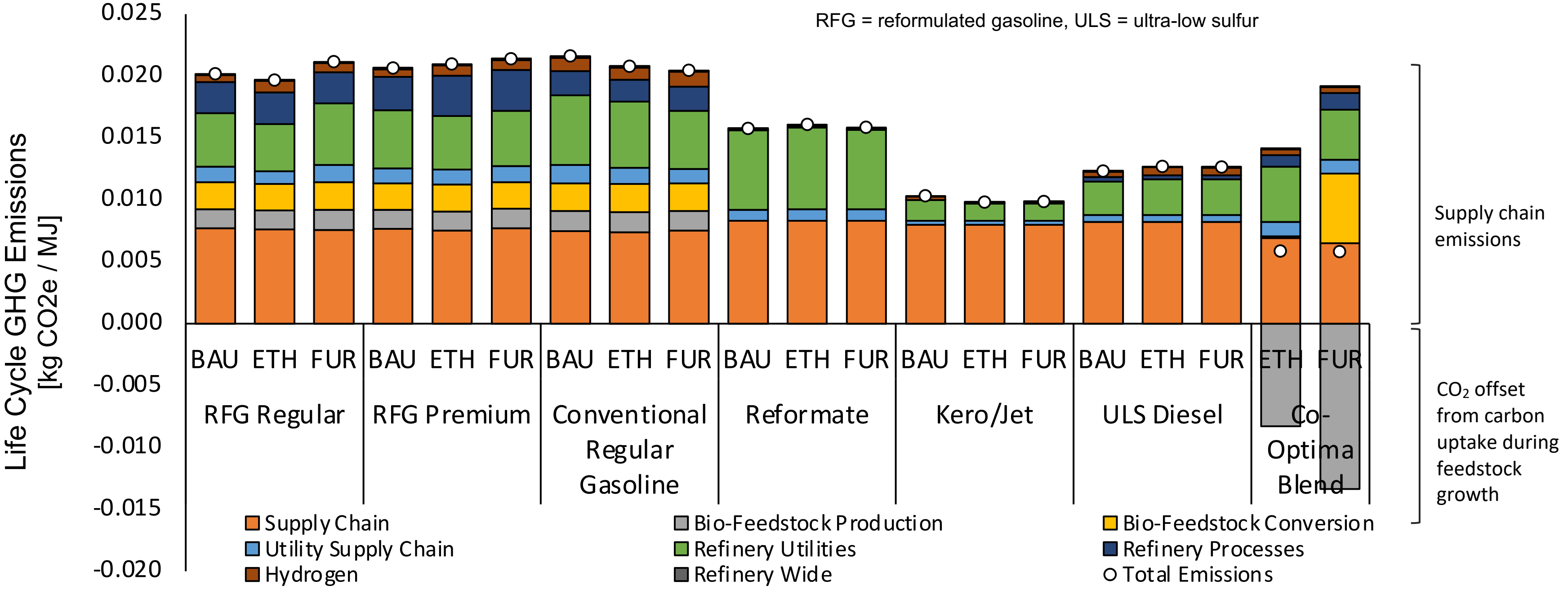
Jiang, Philips, et al. (2021) Fuel; Carlson, Singh, Talmadge, et al. (2021) in prep.

Higher value to smaller, less complex refiners that are octane constrained and produce fewer gasoline varieties

Change over time is due to changing gasoline demand

OUTCOMES GHG reduction in cradle-to-refinery analysis

Biofuels blended at a 20% level, benchmarked against a BAU case



Zaimes, Hawkins, Carlson, et al. (2021) in preparation

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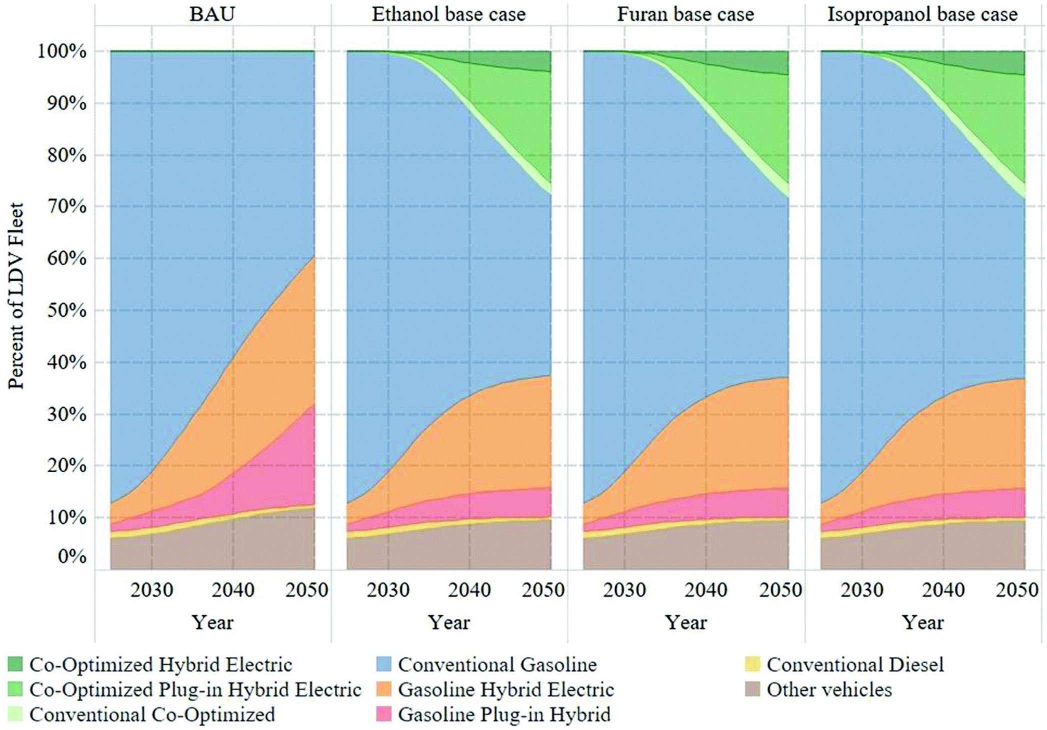
OUTCOMES Adoption of Co-Optima vehicles in the market



Dunn, Newes, Cai et al. (2020) Energy & Environmental Science

Co-optimized vehicles can become future bestsellers by combining better performance and lower fuel cost per mile compared to conventional gasoline and plug-in hybrid electric vehicles (PHEVs)

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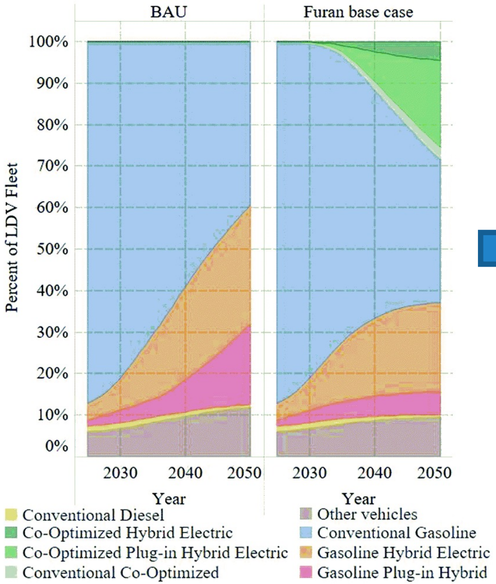
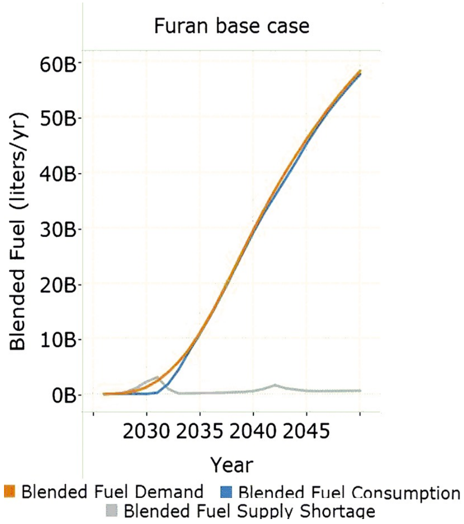
OUTCOMES Adoption to spur biofuel demand, domestic jobs





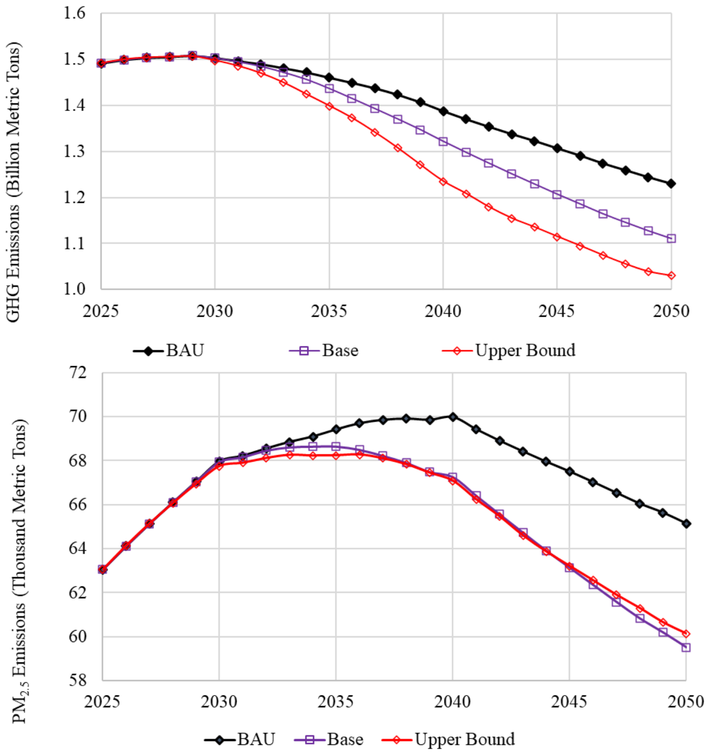
Blended fuel production could achieve 61 billion liters by 2050

Dunn, Newes, Cai et al. (2020) Energy & Environmental Science

Fuel demand estimated from potential fleet evolution using Co-optima engines

Diversifying the fuel resource base leads to significant job creation, esp. in rural areas

OUTCOMES Reduction in GHGs, Criteria Pollutants, Water Use



Biofuel Base and Upper Bound cases, compared to the BAU case

Dunn, Newes, Cai et al. (2020) Energy & Environmental Science

GHGs
- 7% reduction in 2050
- 1.3 billion metric tons

Water
- 9% reduction in 2050
- 2.4 trillion liters

$PM_{2.5}$
- 9% reduction in 2050

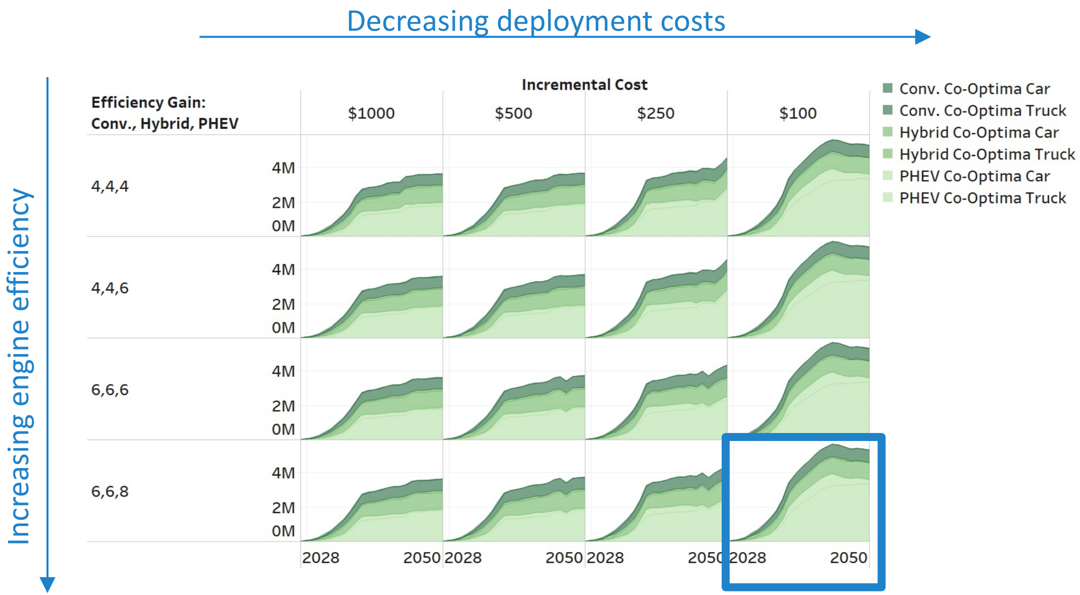
56,000 metric tons

In Progress

Compare synergies with electrification

What tradeoffs between engine efficiency gains vs. incremental vehicle cost influence adoption of co-optimized vehicles with hybridized power trains?

Consider aggressive electrification of the LD passenger fleet?



Sittler, Zaimes, Brooker, Longman et al. (2021) in preparation

Co-Optima: Light Duty Multimode

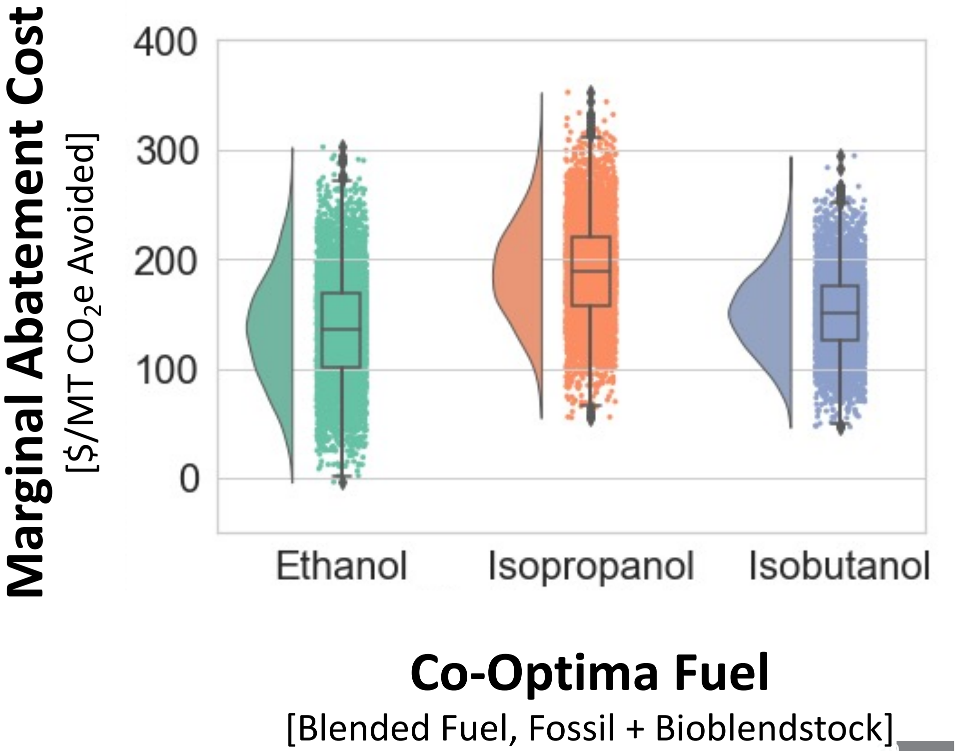
Marginal Abatement Cost (MAC)

Marginal Abatement Cost

- Greenhouse Gas Marginal Abatement Cost (MAC) for Co-Optima Multimode Fuel (RON98), evaluated across three promising bioblendstocks

- Monte-Carlo simulation considers variability in key parameters including:
    - Incremental Vehicle Cost
    - MM Engine Efficiency Gain
    - Gasoline Price
    - Others

- For Co-Optima MM Ethanol, the median (P50) GHG MAC is ~$135/MT-$CO_2$e avoided



Co-Optima Project: Accomplishments

Provide technology options to increase sustainability of transportation

Light Duty

- 10% fuel economy gain over 2015 baseline

Impact

- Petroleum consumption, GHG emissions, water consumption, and $PM_{2.5}$ emissions all reduced when co-optimized fuels and engines emerge

Biofuels

- Diversify resource base (pathways from terrestrial, waste, and algae biomass)
- Provide economic options to adapt to changing demands/sustainability needs
- Increase market opportunities for performance-advantaged biofuels

Crosscutting Goals

- Reduce GHG emissions by at least 20% (demonstrated by a 30% biofuel blend)
- Increase clean energy options and decrease petroleum imports
- Stimulate domestic economy and add new bio-economy jobs

Acknowledgements

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Program Manager, Systems Development & Integration, BETO

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Co-Optima Leadership Team

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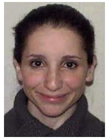
Pacific Northwest National Laboratory



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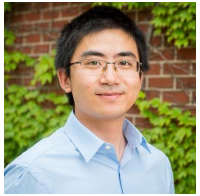
Andrew Bartling


Thathiana Benavides


Aaron Brooker


Hao Cai


Nick Carlson


Scott Curran


Jennifer Dunn


Troy Hawkins


Yuan Jiang


Shuyun Li


Doug Longman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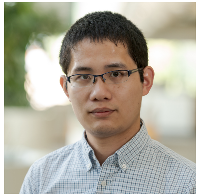
Doris Oke


Longwen Ou


Steve Phillips


Magdelena Ramirez Corredores


Avantika Singh


Lauren Sittler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Ling Tao


Ram Vijayagopal


Yimin Zhang


Greg Zaimes

Including analysis experts representing core capabilities of NREL, ANL, PNNL, ORNL, and INL

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25

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29

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

Bob McCormick
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27

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Avantika Singh
National Renewable Energy Laboratory

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Troy Hawkins
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Magnus Sjöberg
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Robert Wagner
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