Co-Optima Capstone Webinar Series

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

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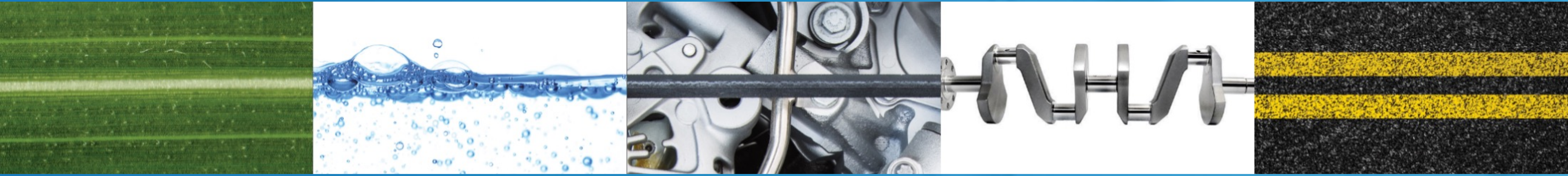
CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



Overview

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

Better fuels. Better engines. Sooner.

Engine R&D

Fuel R&D

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: greenhouse gas [GHG] emissions, toxic emissions)
  - **Low-carbon fuels** (cons: toxic emissions, expensive)

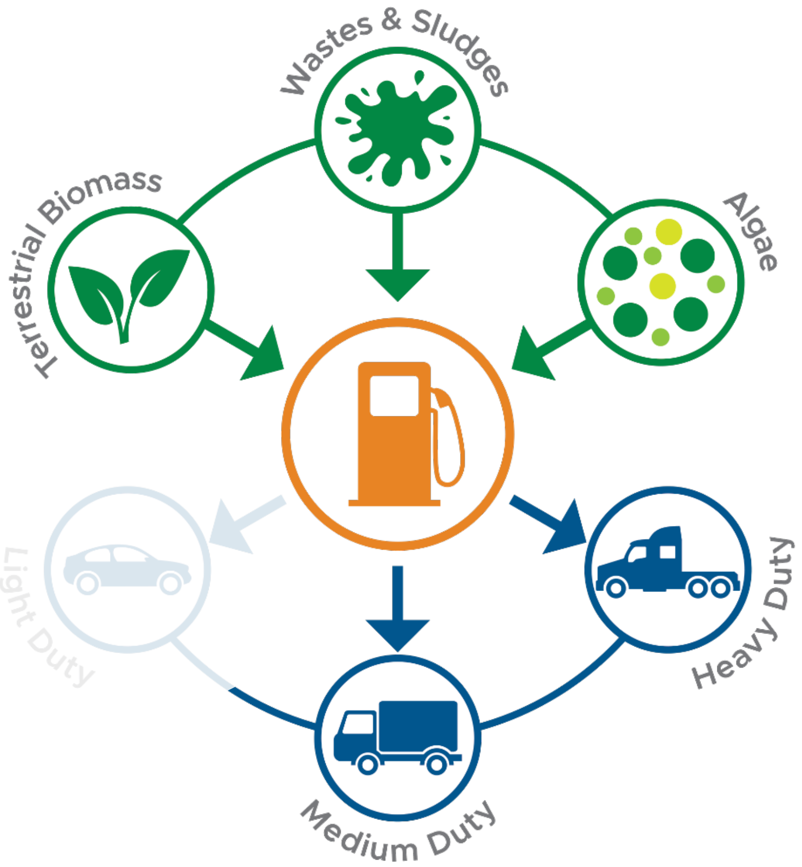
BACKGROUND Why diesel?

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

Image from iStock 182176311

BACKGROUND

Seeking sustainable fuel-engine combinations



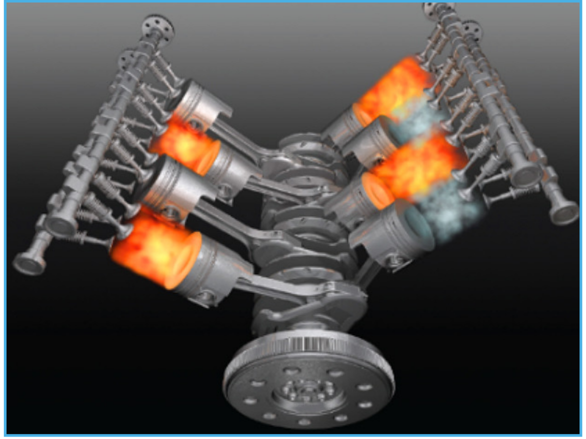
- Focus on liquid fuels
- Identify blendstocks
- Consider non-food-based biofuel feedstocks
- Assess well-to-wheels impacts for biofuel options
- Generate insights on value to refiners, trajectory of vehicle adoption, and socio-economic benefits
- Provide data, tools, and knowledge

Goal

Identify cost-effective, low-carbon drop-in biofuels for diesel engines and quantify their potential costs and benefits at scale.

OBJECTIVE Quantify potential benefits of scaling up

What fuels do engines *really* want?



What fuel options work best?

What will work in the real world?

Photos courtesy of iStock

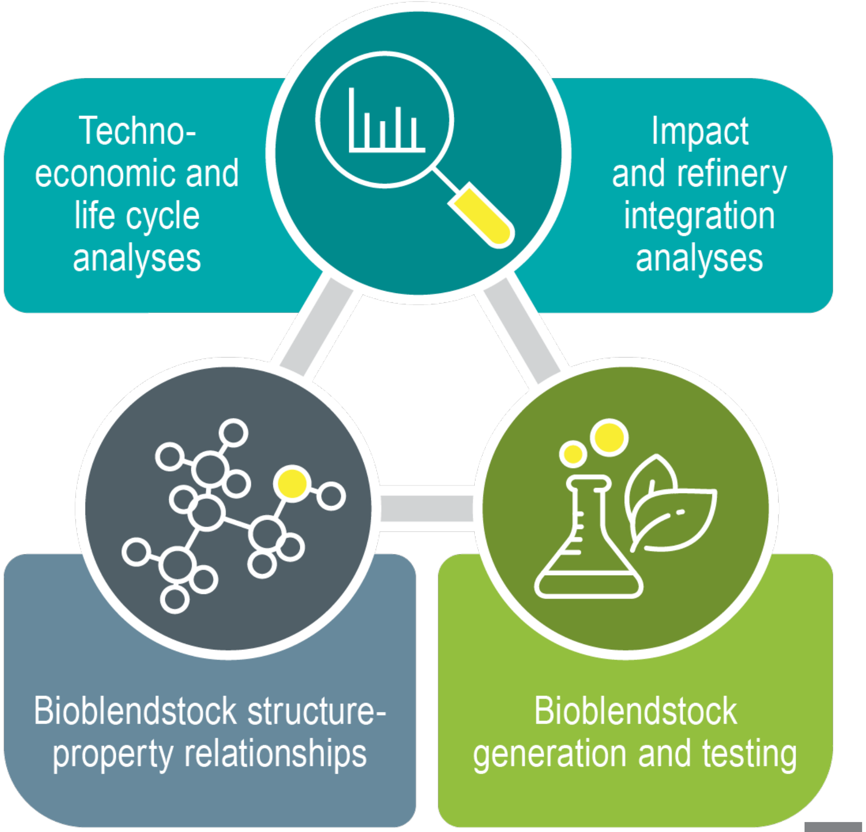
GOAL Inform R&D and commercialization decisions

Goals

- Evaluate selected bioblendstocks.
  - Environmental benefits and tradeoffs
  - Economic drivers
  - Scalability potential
- Quantify benefits and tradeoffs at scale
  - Potential for purchase by consumers
  - Environmental and employment effects

Impact

- Stakeholders understand the costs and benefits of co-optimized fuel-engine strategies and can make informed decisions regarding commercialization and further R&D.



Techno-economic and life cycle analyses

Impact and refinery integration analyses

Bioblendstock structure-property relationships

Bioblendstock generation and testing

Key Takeaways

Low-carbon biofuels could be produced at near-competitive prices to enable clean diesel vehicles

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

- With further development, biofuels for diesel engines could be produced for ~$3-4/GGE with life cycle GHG emissions >60% less than diesel.
- High-cetane, low-sulfur biofuels have potential to drive blending by refiners to meet stringent specifications such as California Diesel Fuel.
- Biofuels and ducted fuel injection have potential to significantly reduce NO_x and PM emissions, enabling clean diesel vehicles.
- Decarbonizing heavy-duty transportation is challenging and costly. Low-carbon biofuels offer a path forward with favorable marginal CO_2 abatement costs.

Research Approach

Quantify the cost and environmental effects of using bioblendstocks in advanced diesel engines. Model vehicle choice and effects at scale.

APPROACH Analysis of costs and benefits across scales

Co-Optimized Biofuels and Compression Ignition Engines for Heavy-Duty Vehicles

Biofuel Production
What are the costs, GHG emissions, and environmental effects of diesel-compatible biofuels?

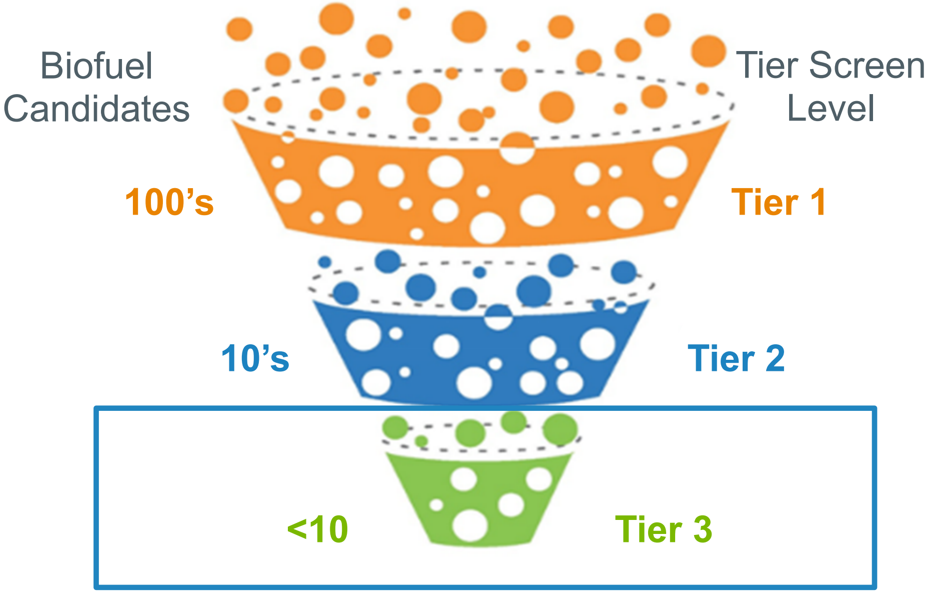
Refinery Benefits
What value can diesel-like biofuels provide the refining industry?

Adoption and Scale Up
How would co-optimized biofuels and engines sell in the heavy-duty market?

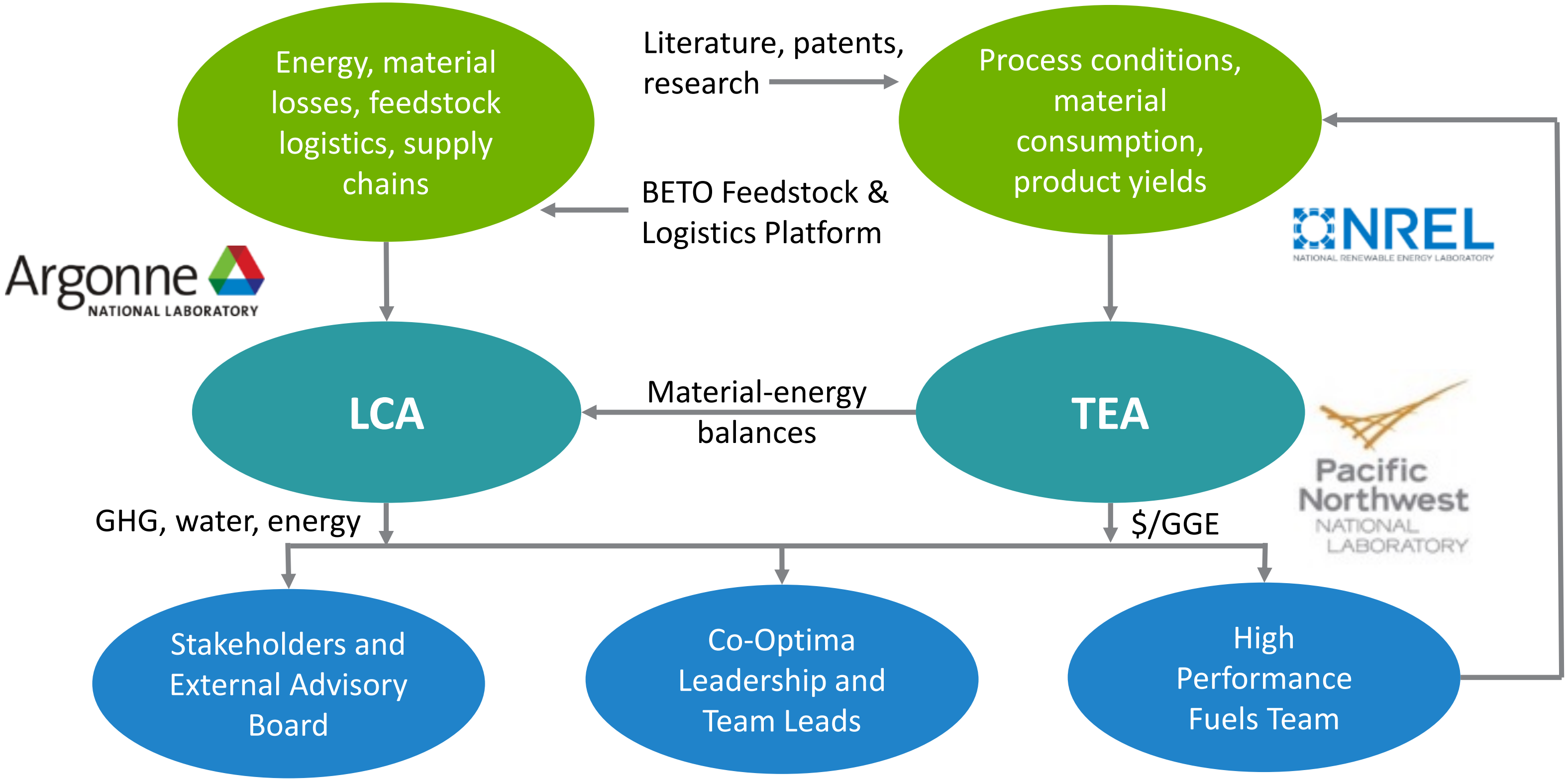
Economy-wide Benefits
What are the environmental and societal effects of heavy-duty biofuels and engines at scale?

APPROACH Select fuel pathways to evaluate

- Down-select performance-enhancing fuels
    - Based on properties from Advanced Engine Development and Fuel Properties teams
- Select promising feedstocks
- Develop process models
    - In consultation with High Performance Fuels team.
    - Consider a diverse set of production methods, chemical structures, and feedstocks.
- Calculate key metrics
    - Minimum fuel selling price (MFSP)
    - GHG emissions
    - Water use
    - Energy use



APPROACH TEA and LCA inform research direction



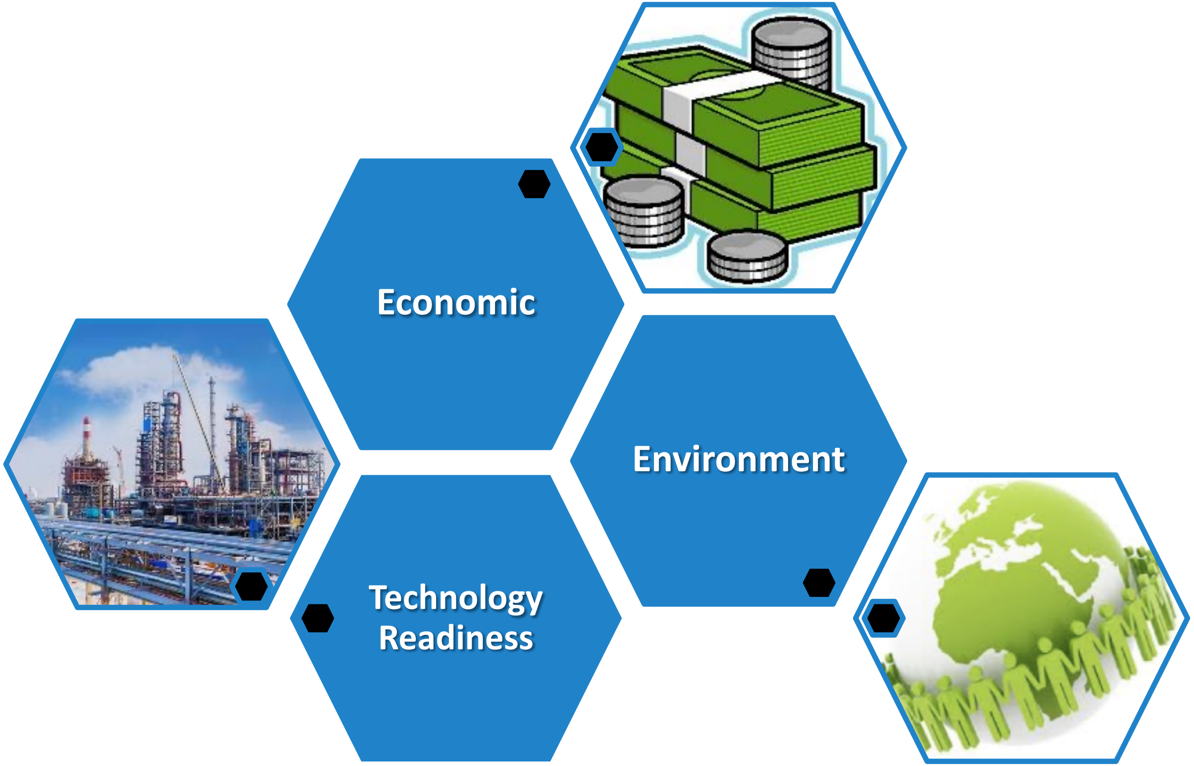
BETO = Bioenergy Technologies Office, GGE = gasoline gallon equivalent, LCA = life cycle analysis, TEA = techno-economic analysis

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



APPROACH

Evaluate biofuels against cost, environmental, and scalability considerations

Cost Metrics - TEA

Baseline cost

Target cost

Baseline-to-target cost ratio

% of price dependent on co-products

Market competition for the bioblendstock and precursors

Feedstock cost

Environmental Metrics – LCA

Carbon efficiency, baseline

Carbon efficiency, target

Conversion yield, baseline, GGE/dry ton feedstock

Conversion yield, target, GGE/dry ton feedstock

Life-cycle GHG reduction compared with conventional fuel, target

Life-cycle fossil energy reduction compared with conventional fuel, target

Life-cycle water consumption

Scalability Metrics

Process modeling data source

Sensitivity of production process to feedstock type

Conversion robustness to feedstock variability

Blending behavior with conventional fuel

Bioblendstock underwent testing towards certification

Legal limits to blend level

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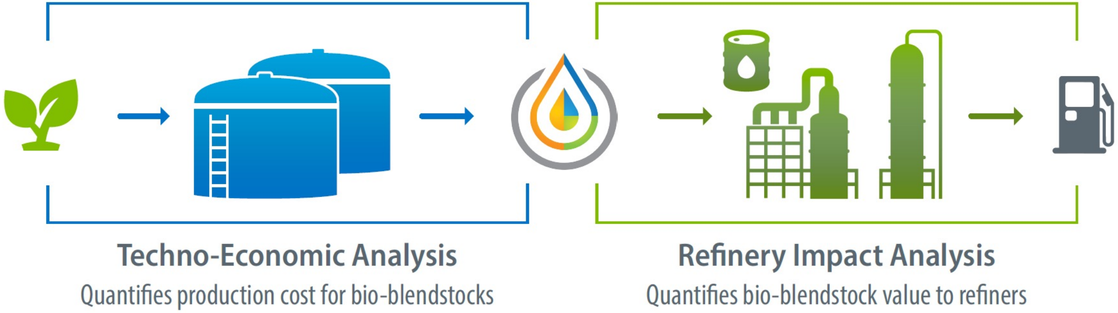
APPROACH Refineries reoptimize to blend biofuels



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

Effect re-optimization on unit operations

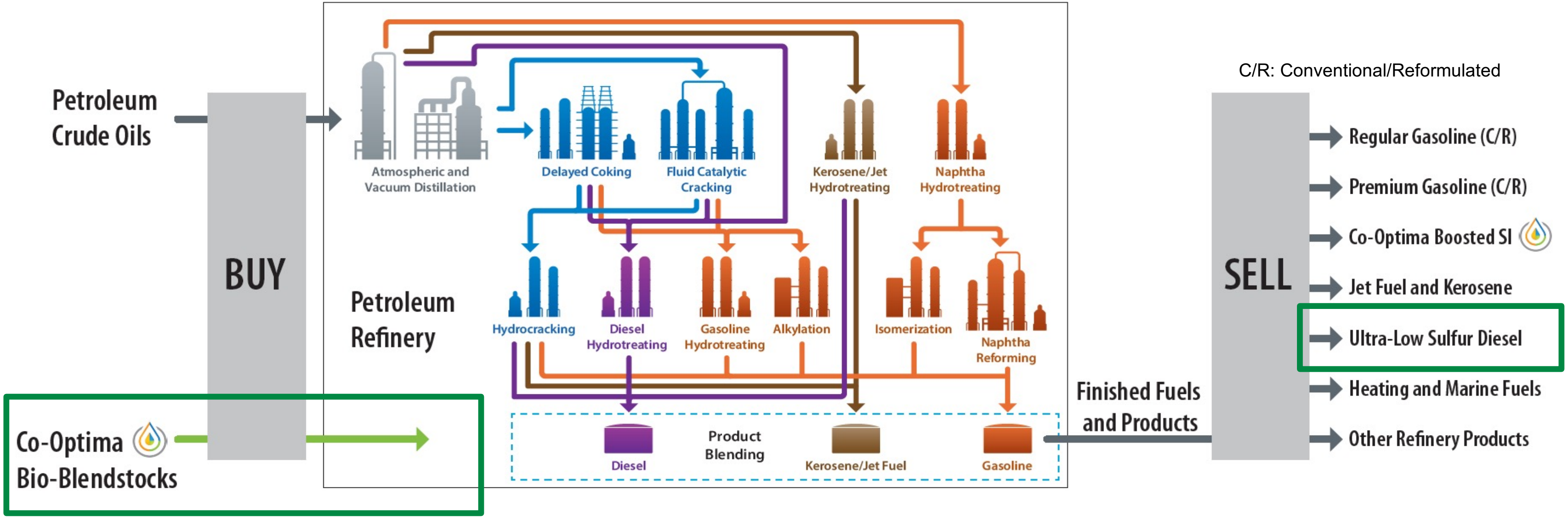
Overview of Commercial Refinery Modeling Scope in Aspen PIMS

Crude oil quality data (assays)

Pricing models for crude oils as functions of quality

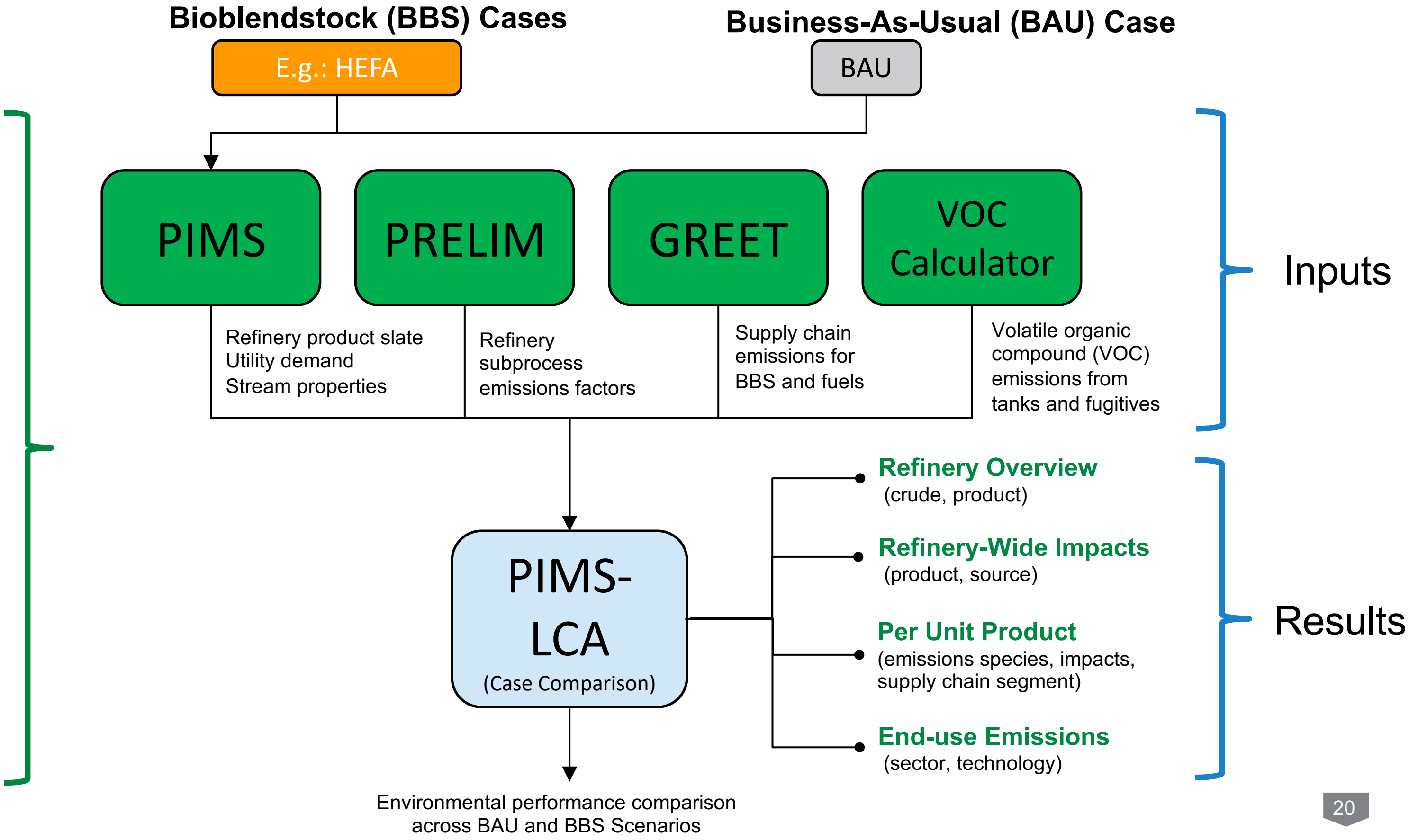
Quality specifications for finished fuels

Pricing models for finished fuels and co-products



APPROACH Coupled LCA to model environmental impact

Excel-based tool to inform carbon intensity of refinery emissions



Bioblendstock (BBS) Cases

E.g.: HEFA

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, impacts, supply chain segment)

End-use Emissions
(sector, technology)

Results

Environmental performance comparison across BAU and BBS Scenarios

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APPROACH HD fleet projected by vehicle choice model

1. Scenarios start with all existing Class 8 tractor options

- Captures diversity of performance characteristics & pricing

ADOPT

2. New vehicles introduced to market based on best-sellers

- Trade-offs made in vehicle attributes based on the relative value to consumers

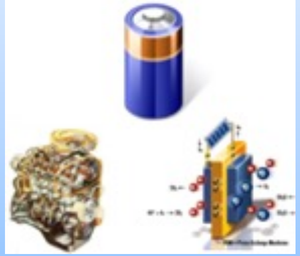
3. Sales estimates are used for future vehicle evolution

- Process iterates through 2050
- Component sizing is optimized using FASTSim

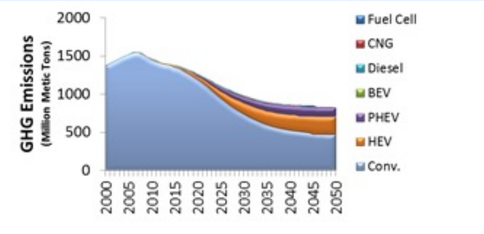
FASTSim

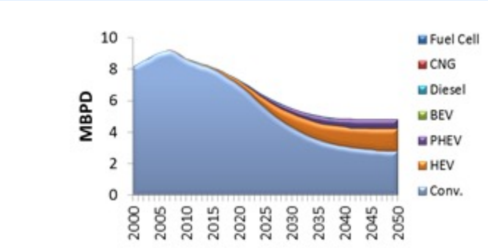
4. Sales placed into a stock model to estimate total fleet GHG emissions and petroleum consumption

Technical Targets



Vehicle Emissions and Energy Consumption





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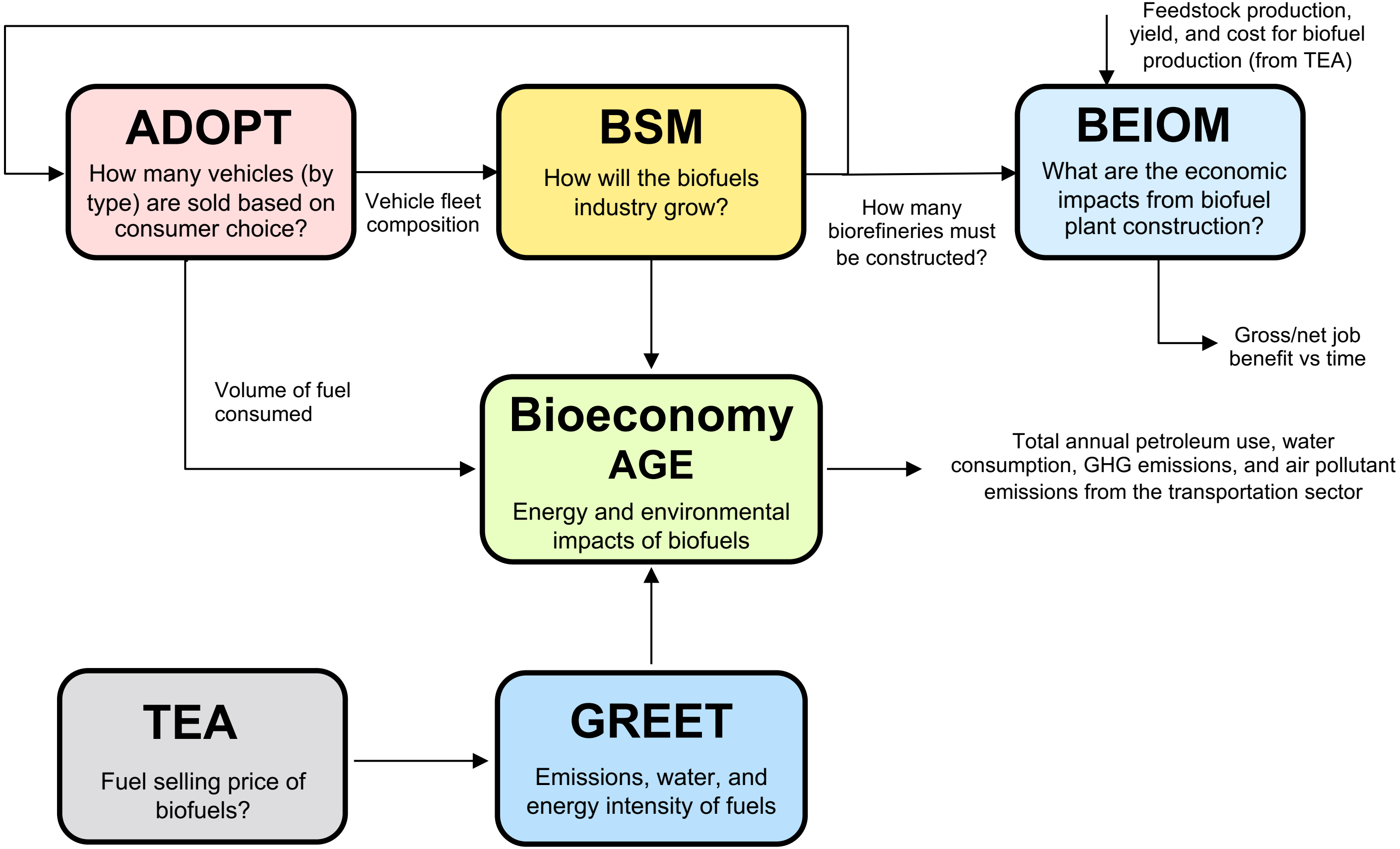
APPROACH Integrated tools evaluate cumulative benefits



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

- Low-carbon biofuels could be produced at near-competitive prices.
- There is potential for market pull by refiners.
- Biofuels can reduce GHGs for trucks already on the road, while advanced engines have additional NO_x/PM benefits.

OUTCOMES Environmental, cost, and scalability metrics

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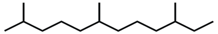
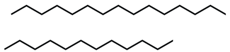
OUTCOMES Screening identified 13 promising MCCI biofuels

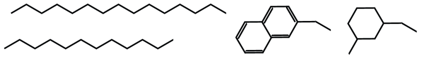
Hydrocarbons



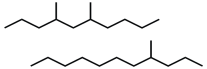
farnesane



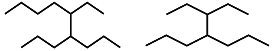
Fischer-Tropsch diesel



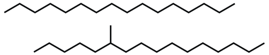
hydrothermal liquefaction oil from wet waste, algae, and algae-wood blends



isoalkanes made from ethanol

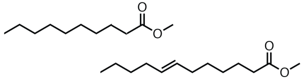


isoalkanes via volatile fatty acids from food waste

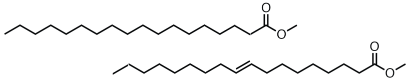


hydroprocessed esters and fatty acids (renewable diesel)

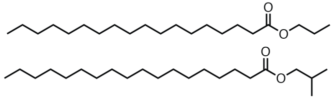
Esters



short chain esters from oilseed crops

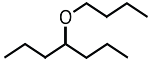


fatty acid methyl esters/biodiesel

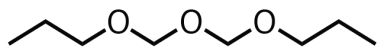


fatty acid fusel esters

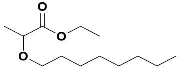
Ethers



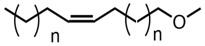
4-butoxyheptane



polyoxymethylene ethers (POMEs)



alkoxyalkanoates



fatty alkyl ethers

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

		Technology Readiness						Economic Viability						Environmental							Totals			
		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[4]	Baseline carbon efficiency	Target carbon efficiency	Baseline yield[5]	Target yield[5]	LC GHG[4]	LC fossil[4]	LC water[4]	🟢	🔵	🟠	⚪
Biochemically-Based Pathways	Long Chain Primary Alcohols	🔵	🟢	🔵	⚪	⚪	⚪	🟠	🟠	🟠	🟢	🟢	🟢	🟠	🟠	0.3	27	🟠	🟠	🔵	4	3	7	3
	Alkoxyalkanoate Ether-Esters	🔵	🟢	🔵	⚪	⚪	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🔵	🔵	51	71	🟢	🟢	🔵	9	5	0	3
	4-Butoxyheptane	🔵	🔵	🔵	🔵	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	40	47	🟠	🔵	🔵	4	8	3	2
	Mixed Dioxolanes	🔵	🔵	🔵	⚪	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	43	43	🟠	🟠	🔵	4	6	4	3
	5-Ethyl-4-Propyl-Nonane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟠	35	45	🟠	🔵	🔵	4	8	3	2
	4-(Hexyloxyl)Heptane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🟠	🟢	🟢	🟢	🟢	🔵	🟠	43	47	🟠	🔵	🔵	4	7	4	2
	Farnesane*	🔵	🔵	🔵	🟢	🟢	🔵	🟠	🔵	🔵	🔵	🟢	🟢	🔵	🟠	30	43	🟢	🟢	🔵	6	9	2	0
	n-Undecane	🔵	🔵	🔵	🟢	⚪	🟢	🟠	🔵	🔵	🟢	🟢	🟢	🟠	🟠	9	47	🟠	🔵	🔵	5	7	4	1
	Hexyl-Hexanoate	🔵	🔵	🔵	⚪	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🟠	🔵	9	49	🟠	🔵	🔵	4	7	3	3
	Isoalkanes from Volatile Fatty Acids	🔵	🟠	🟠	🟢	🟢	🟢	🔵	🔵	🟢	🟢	🟢	🟢	🟠	🔵	31	42	🟢	🟢	🔵	9	5	3	0
	Cyclopropanes	🔵	🔵	🔵	🟢	⚪	🟢	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟢	39	67	🟠	🔵	🔵	7	7	2	1
	Bicyclohexane	🔵	🟢	🔵	🟢	⚪	🟢	🟠	🟠	🟢	🟢	🔵	🟢	🟠	🟠	30	33	🟠	🟠	🔵	6	4	6	1
Thermochemical Pathways	**Renewable Diesel via HTL of Wet Wastes**	🔵	🟢	🟢	🔵	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	95	107	🟢	🟢	🟢	14	2	0	1
	Renewable Diesel via HTL of Whole Algae	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🔵	🟢	🟢	🟠	🟢	🟢	83	130	🟢	🟢	🔵	6	7	2	2
	Renewable Diesel via HTL of Whole Algae/Wood Blend	🔵	🔵	🔵	🔵	⚪	⚪	🟢	🟢	🟢	🟢	🟢	🟠	🟢	🟢	70	130	🟢	🟢	🟠	9	4	2	2
	Long Chain Mixed Alcohols	🔵	🟢	🟢	⚪	⚪	⚪	🟢	🔵	🟢	🟢	🟢	🟢	🔵	🟠	42	42	🔵	🟢	🔵	8	5	1	3
	One-Step POMEs from Methanol	🟠	🟢	🟢	🔵	⚪	⚪	⚪	🔵	⚪	🟢	🟢	🟢	⚪	🔵	⚪	52	🟢	🟢	🔵	7	4	1	6
	Fischer-Tropsch Diesel	🟢	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🟢	🟠	🟢	🟢	🔵	🟠	32	32	🟢	🟢	🔵	12	3	2	0
Catalytic/Hybrid Pathways	**Biodiesel (FAME)***	🟢	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🟠	🟠	🟢	🟢	>200		🟢	🟢	🟠	13	1	3	0
	Hydroprocessed Esters and Fatty Acids (HEFA)[2]	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🟠	🟠	🟢	🟢	171	171	🟢	🟢	🟢	14	1	2	0
	Fatty Alkyl Ethers[1]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	232	290	🟢	🟢	🔵	8	5	2	2
	Fatty Alkyl Ethers[2]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🟢	🟢	🟢	🟠	🟠	🟢	🟢	210	263	🟢	🟢	🟢	10	3	2	2
	Fatty Alkyl Ethers[3]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	246	308	🔵	🟢	🟠	7	5	3	2
	Short-Chain Esters from Oilseed Crops	🟢	🟢	🟢	🟢	🟢	🔵	🟠	⚪	⚪	🟢	🟠	🟠	🟢	🟢	258	258	⚪	⚪	⚪	8	1	3	5
	Fatty Acid Fusel Esters	🔵	🟢	🟢	⚪	⚪	🔵	🟢	🟢	🟢	🟢	🔵	🟠	🟢	🟢	143	185	🔵	🟢	🟠	9	4	2	2

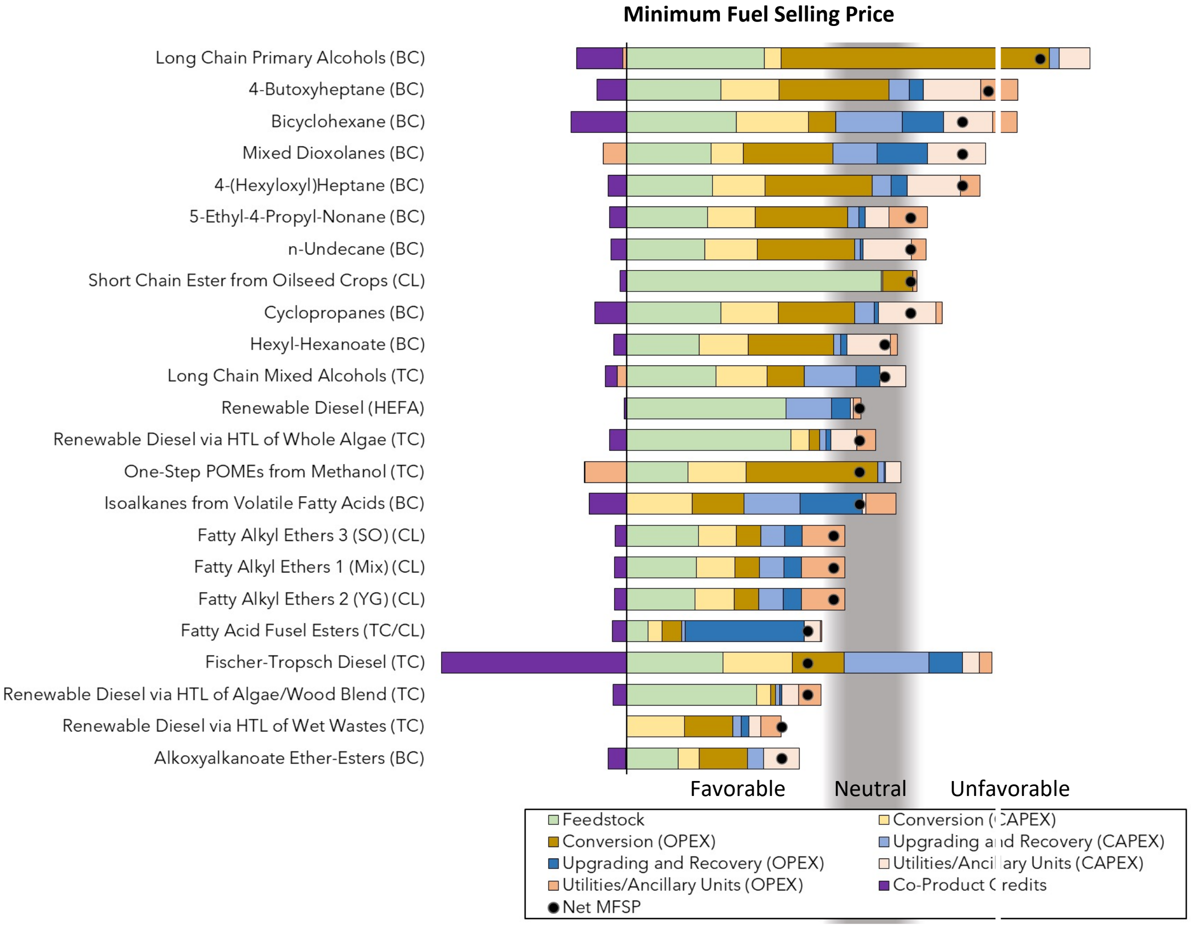
OUTCOMES Reducing cost is a key challenge

Feedstock costs contribute significantly to MFSP
  - Identifying waste pathways could reduce cost

Conversion costs highest for biochemical pathways
  - Caustic used in pretreatment
  - Glucose used in enzyme production

Co-product credits are typically low

Upgrading and recovery costs typically low



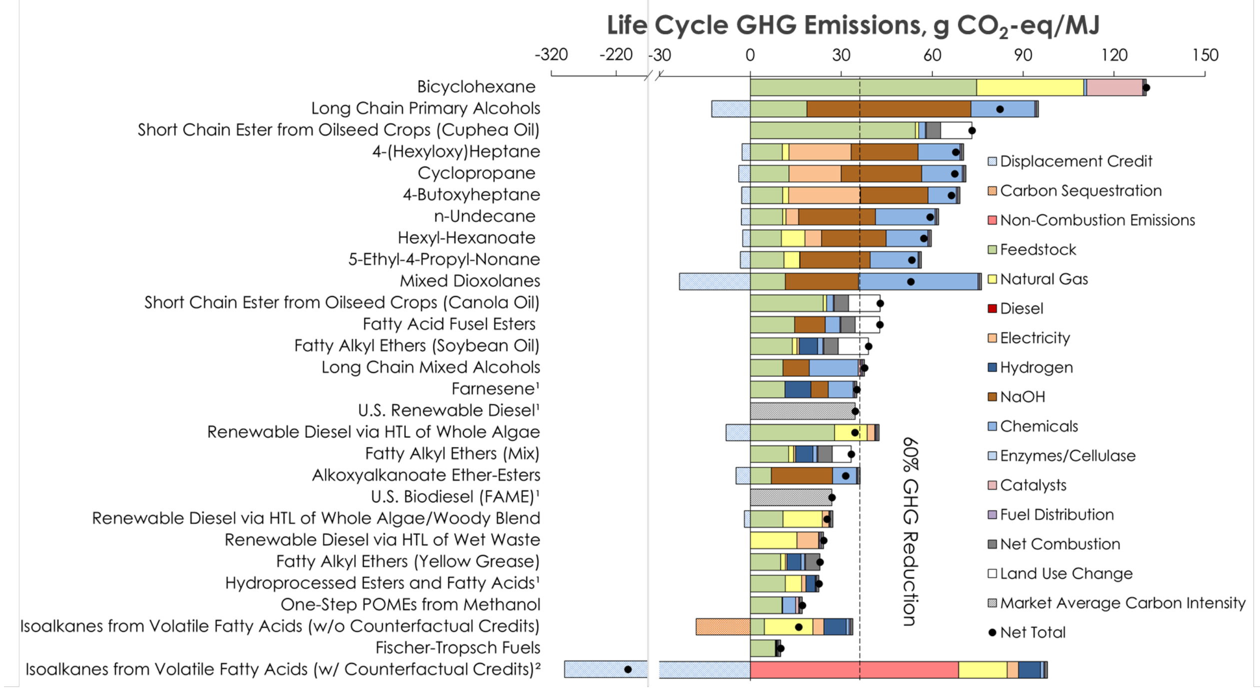
OUTCOMES Potential for significant GHG reductions

…but not guaranteed for all biofuels

Variety of feedstocks and pathways could provide low-carbon MCCI fuels

Opportunities to improve GHG emissions

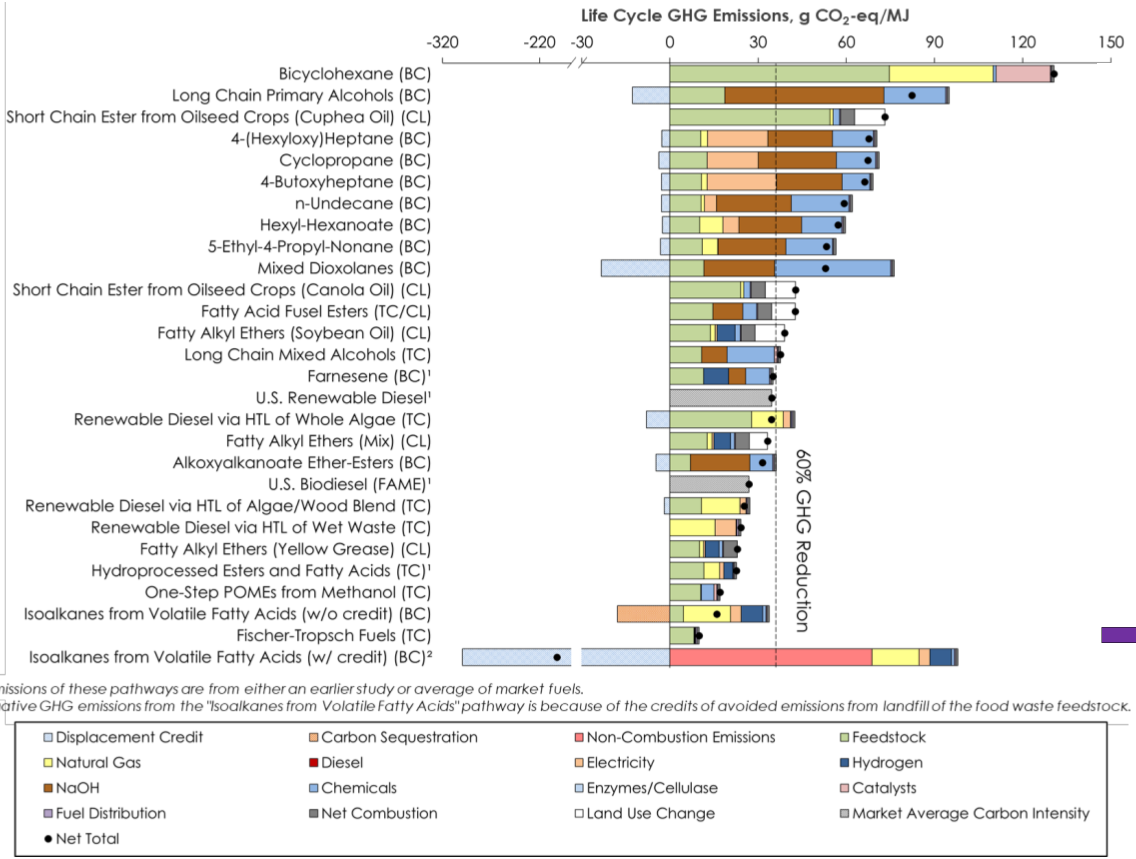
- Feedstock production
- NaOH for feedstock pretreatment
- Chemical inputs



[1] GHG emissions of these pathways are from either an earlier study or average of market fuels.

[2] 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 Potential for significant GHG reductions



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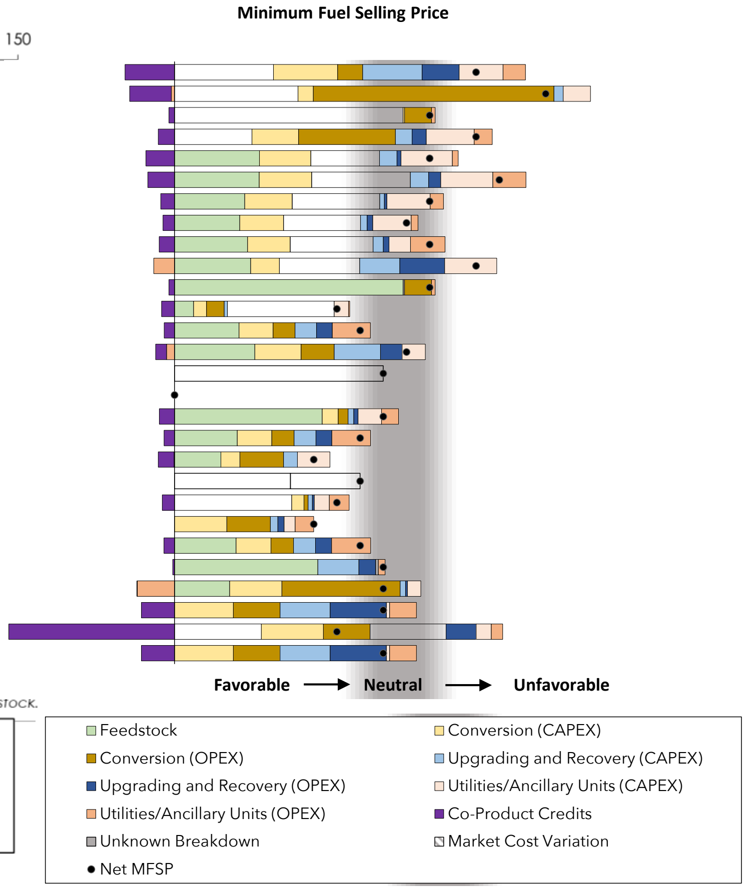
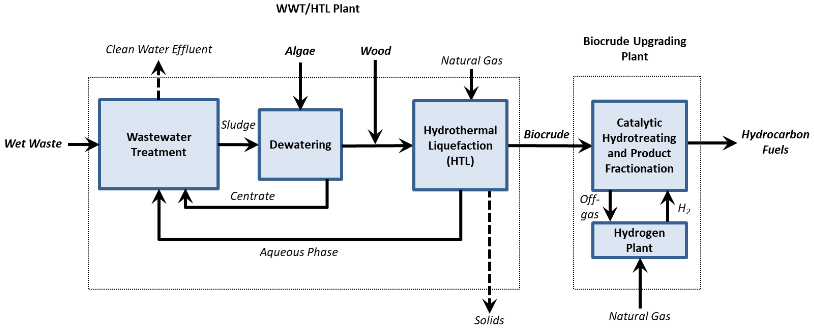
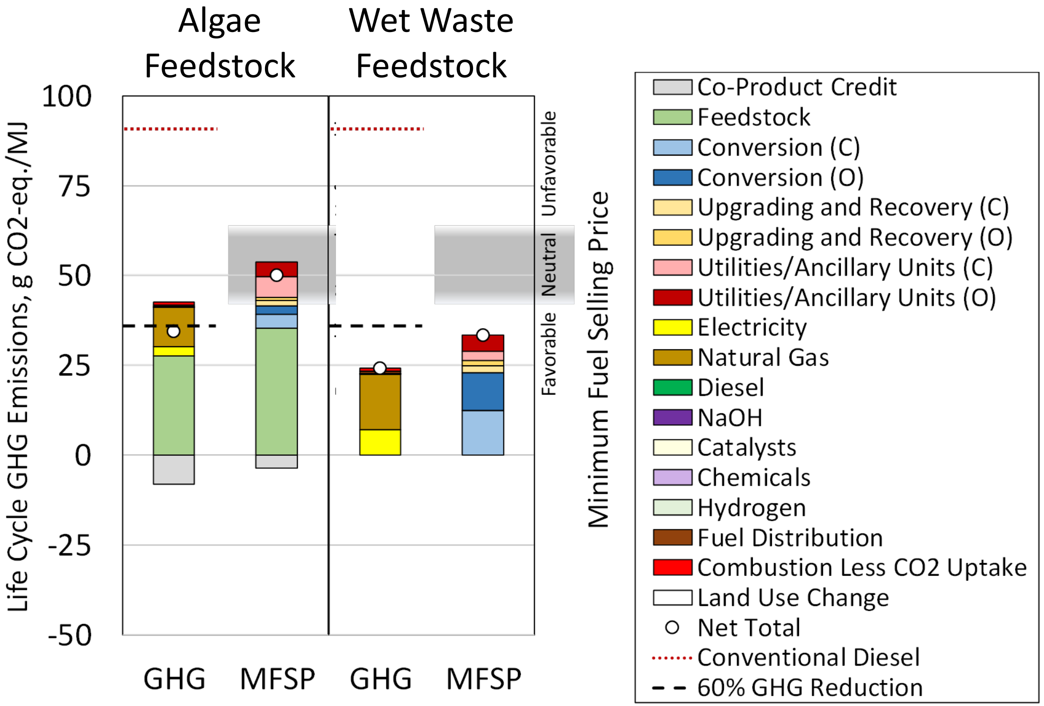


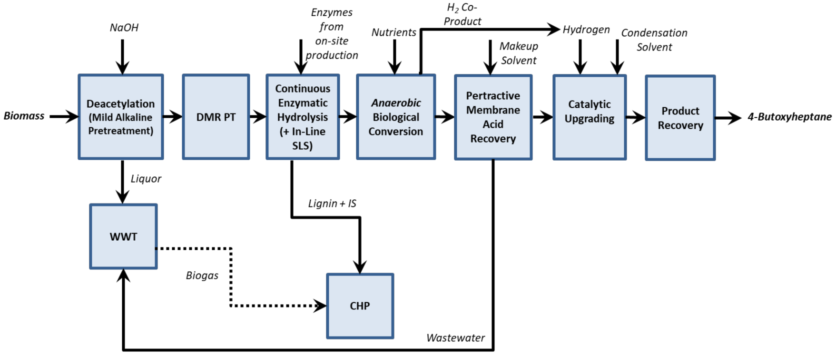
OUTCOMES Opportunity for hydrothermal liquefaction

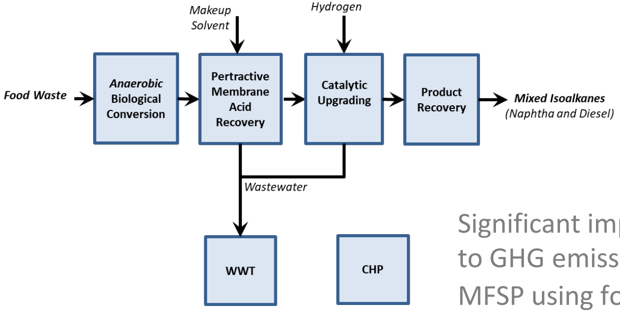




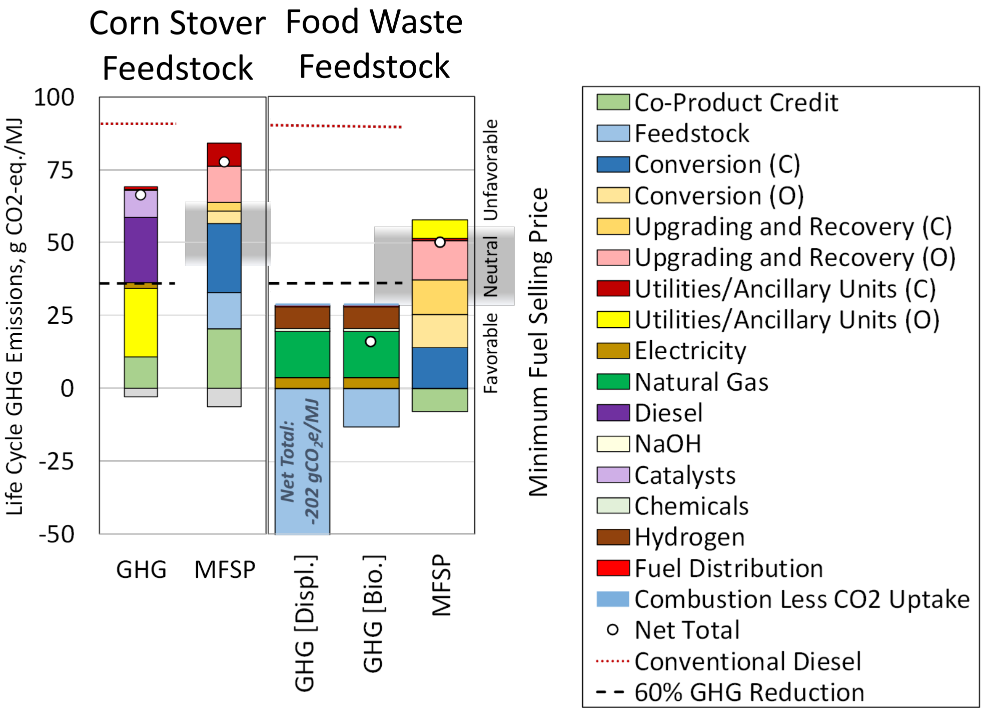
Comparison of life-cycle GHG emissions and MFSP breakdowns for two HTL pathways. Using wet waste feedstocks (right) can significantly reduce both cost and emissions versus algae (left) or lignocellulosic feedstocks.

OUTCOMES Isoalkanes and acids pathways





Significant improvements to GHG emissions and MFSP using food waste



OUTCOMES

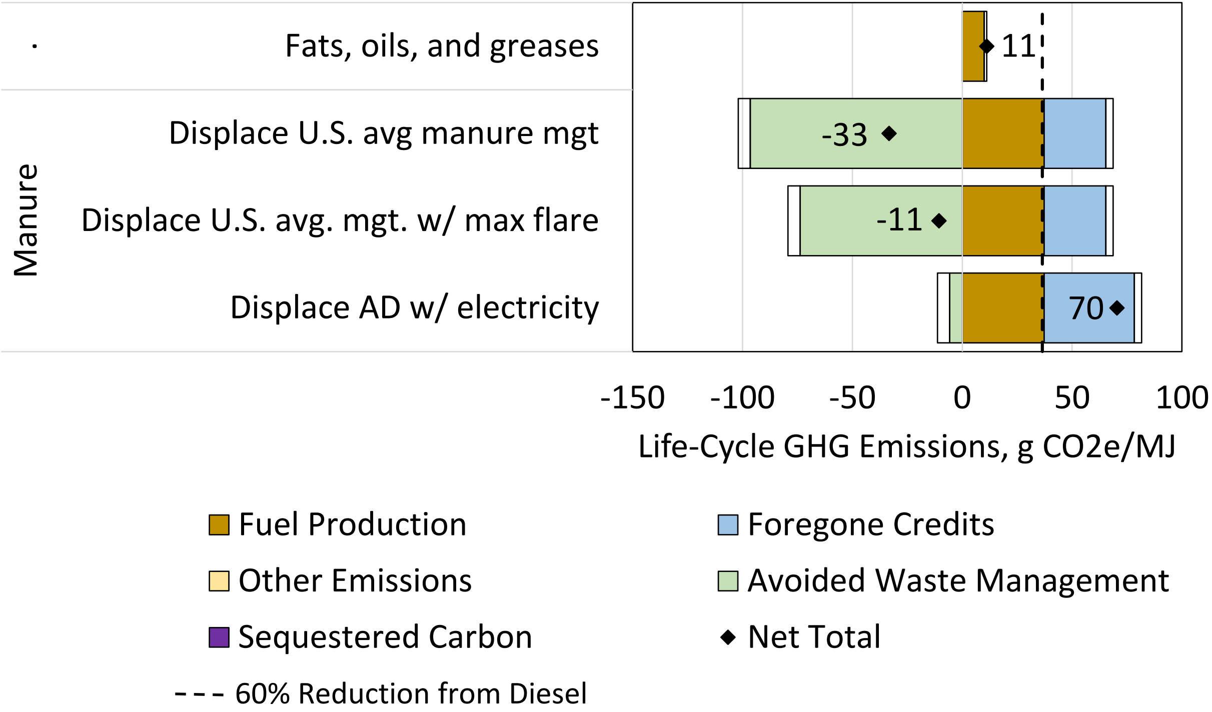
Renewable diesel from waste with very low GHGs for less than $4.50/GGE

Hydrothermal liquefaction of swine manure

- GHG reduction >100%
  due to avoided emissions from manure management
- MFSP ~$3.60/gge
  drops to $3.10/gge when scaled to 250 tonnes/day

Hydroprocessing of fats, oils, & greases

- GHG reduction ~87%
- MFSP ~$4.40/gge
  potentially lower at larger scale



OUTCOMES Value of biofuels for refining industry

Co-Optimized Biofuels and Compression Ignition Engines for Heavy-Duty Vehicles

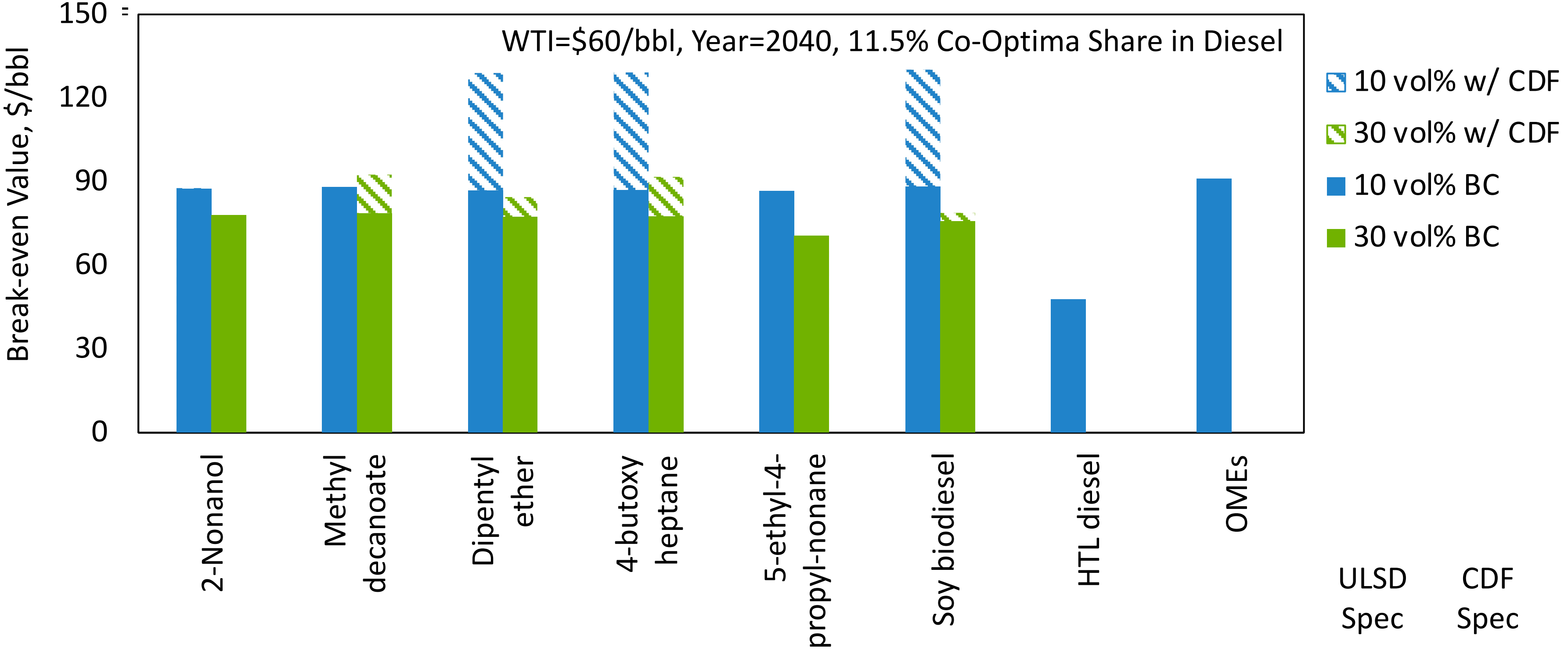
Biofuel Production
What are the costs, GHG emissions, environmental effects, and scalability of diesel-compatible biofuels?

Refinery Benefits
What value can diesel-like biofuels provide the refining industry?

Adoption and Scale Up
Would co-optimized biofuels and engines sell in the heavy-duty market?

Economy-wide Benefits
What are the environmental and societal effects of heavy-duty biofuels and engines at scale?

OUTCOMES Diesel bioblendstocks could add value for refineries



	2-Nonanol	Methyl decanoate	Dipentyl ether	4-butoxy heptane	5-ethyl-4-propyl-nonane	Soy biodiesel	HTL diesel	OMEs	ULSD Spec	CDF Spec
Cetane #	38-41	46-52	91-96	57-65	48	54-55	65.8	93	>40	>53

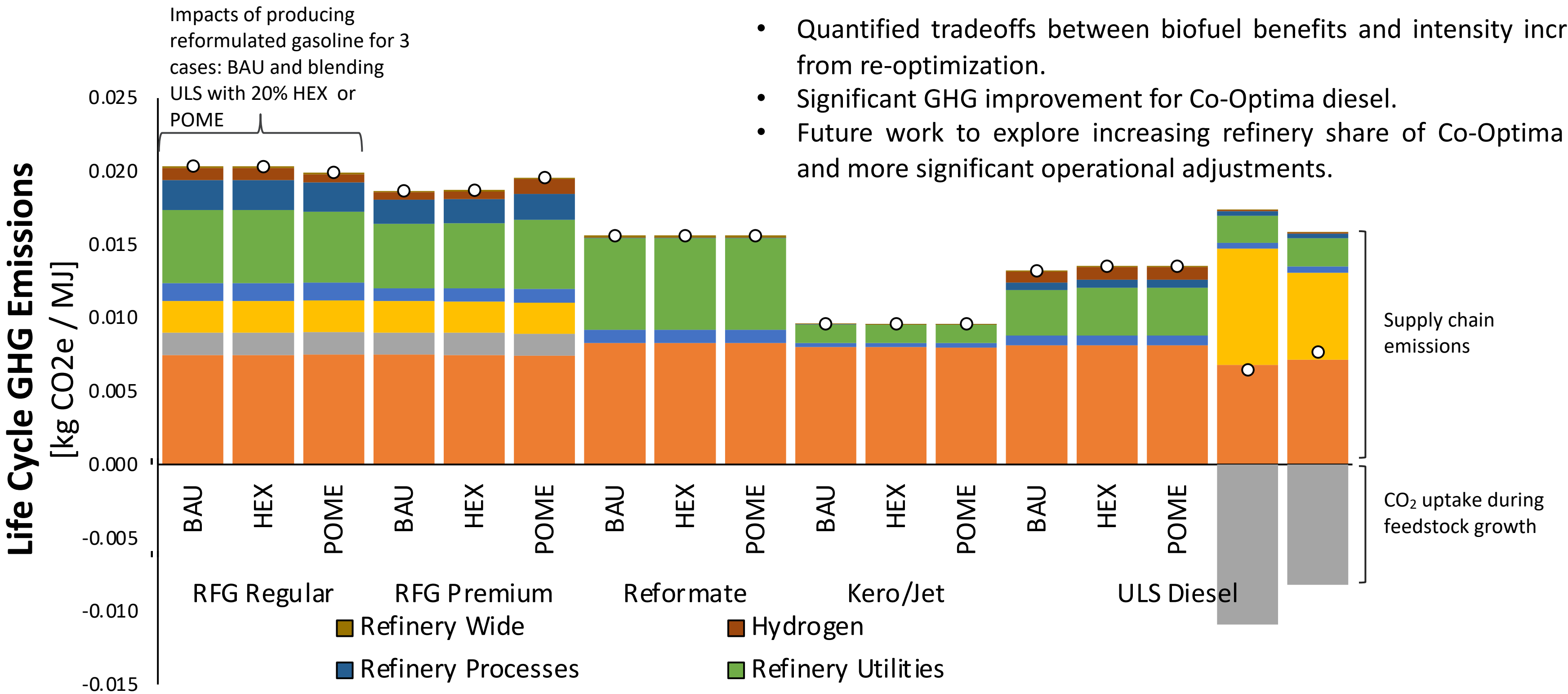
Property criterion: **Greatly Exceeds**, **Exceeds Criteria**, **Meets Criteria**.

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

OUTCOMES

GHG benefits of blending Co-Optima fuels outweigh potential tradeoffs

Cradle-to-refinery gate GHG results for a large refinery configuration, $60/BBL oil price (WTI), 20% volume blend of hexyl hexanoate (HEX) and POME compared with business as usual (BAU)



- Quantified tradeoffs between biofuel benefits and intensity increases from re-optimization.
- Significant GHG improvement for Co-Optima diesel.
- Future work to explore increasing refinery share of Co-Optima fuels and more significant operational adjustments.

OUTCOMES Adoption and scale up

Co-Optimized Biofuels and Compression Ignition Engines for Heavy-Duty Vehicles

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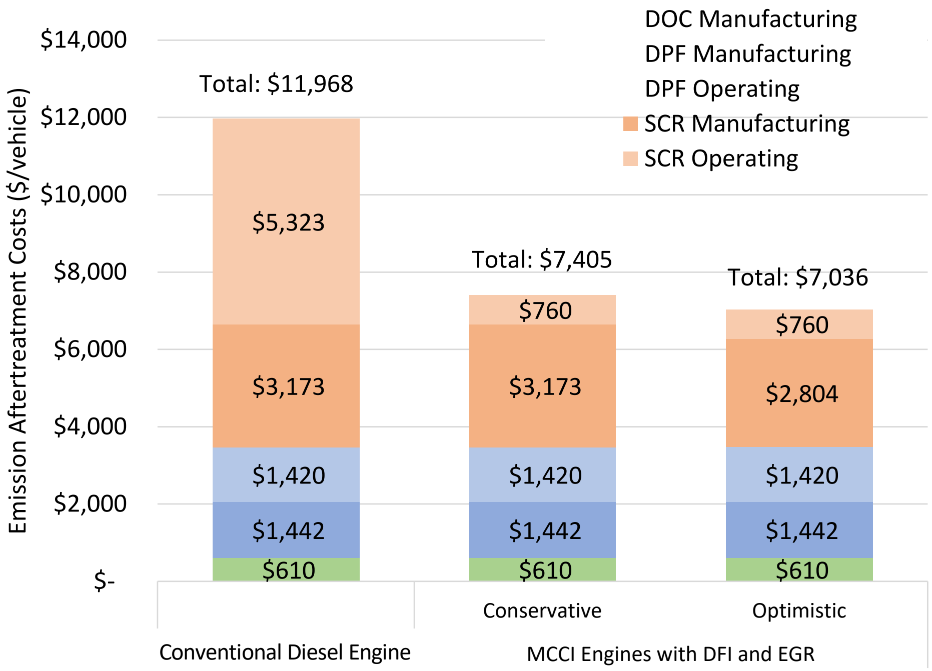
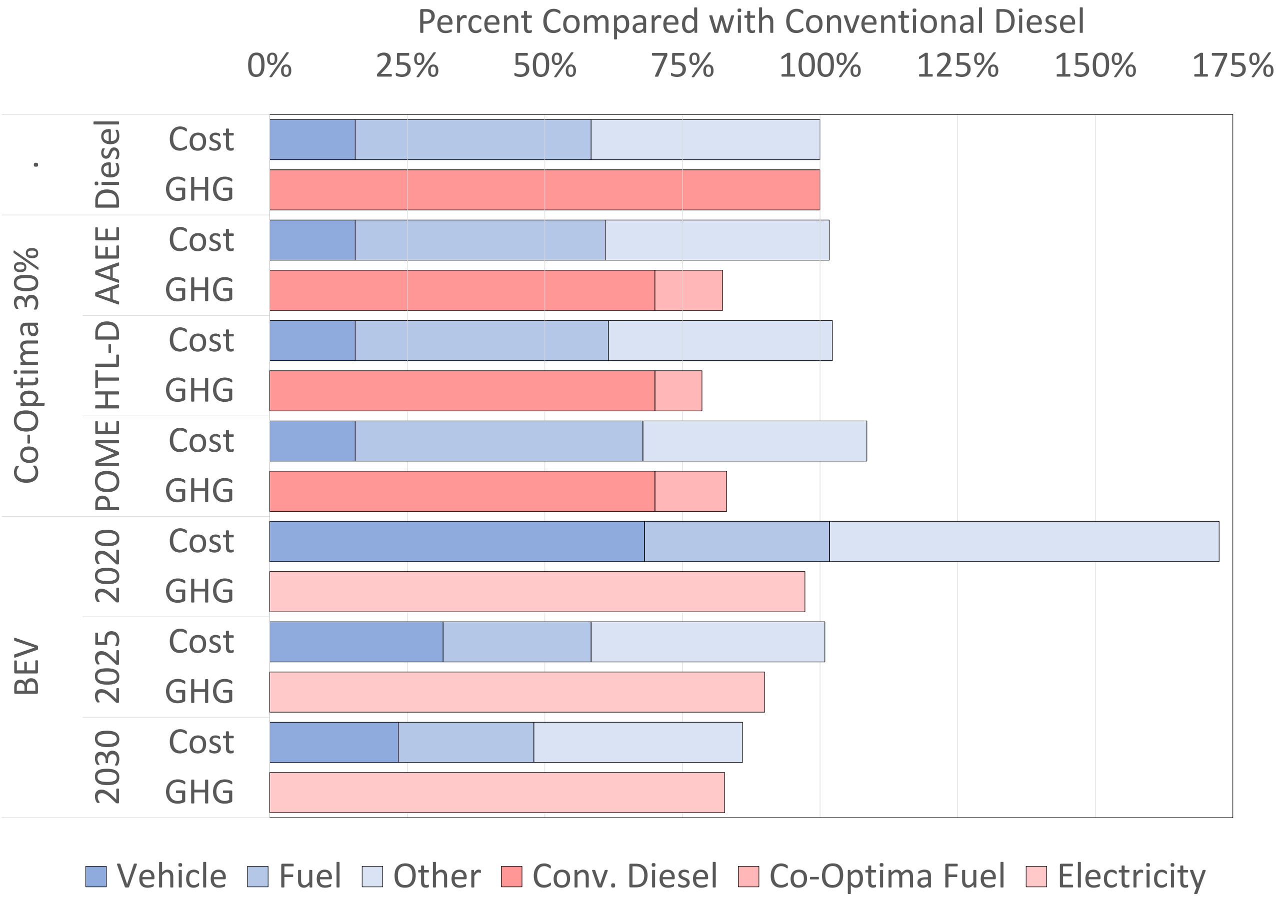
OUTCOMES Reduced NO_x and PM control costs

- >80% reductions in engine-out NO_x and PM
- $4,500-$5,000 lifetime cost reduction
  - Reduced use of exhaust fluid
  - Downsizing selective catalytic reduction system



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

OUTCOMES Drop-in biofuels reduce GHGs from today's fleet

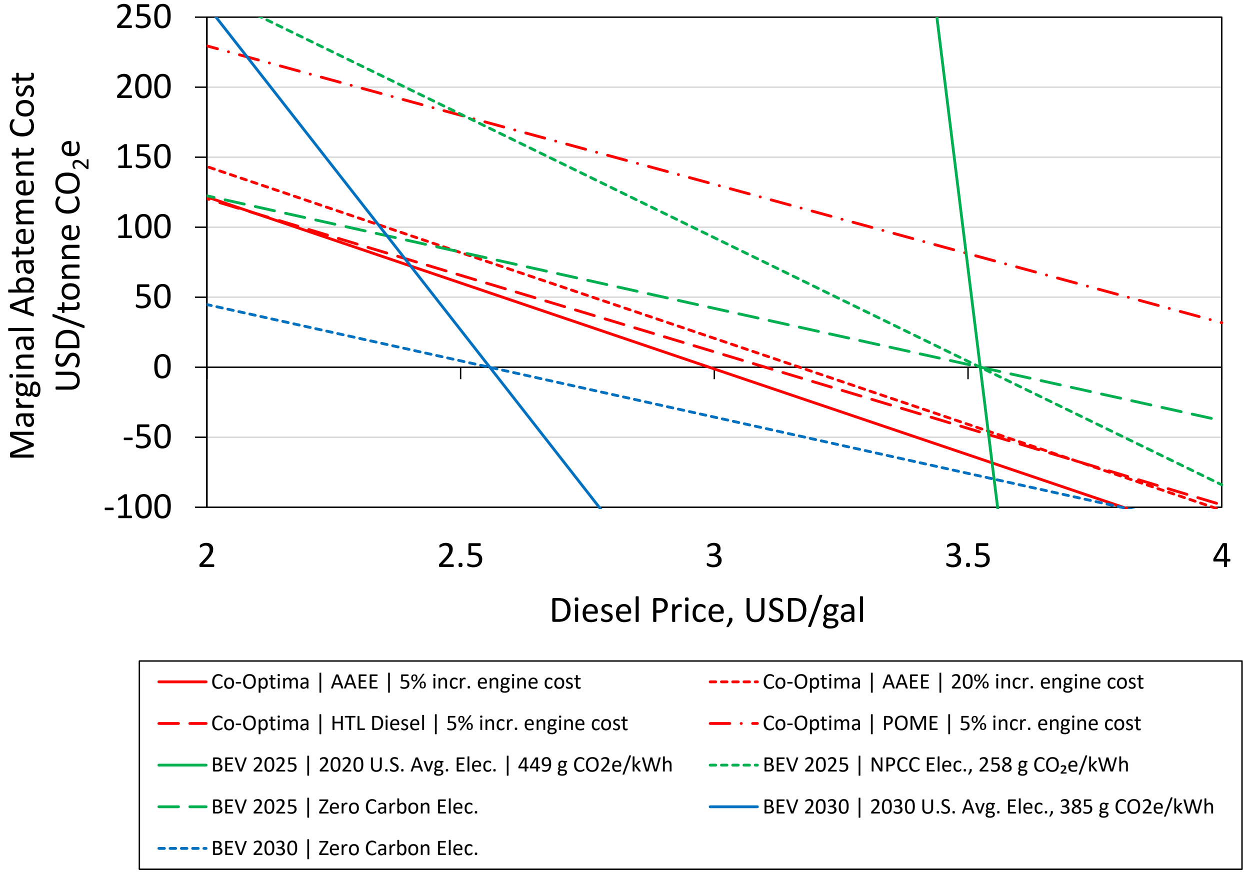


…and PM/NOx reductions in co-optimized engines

At a cost that's competitive with electric trucks in the near-term

OUTCOMES

Biofuels offer attractive GHG abatement costs for heavy-duty vehicles



Biofuels and electrification could offer complimentary strategies for distinct applications

OUTCOMES Adoption and scale up

Co-Optimized Biofuels and Compression Ignition Engines for Heavy-Duty Vehicles

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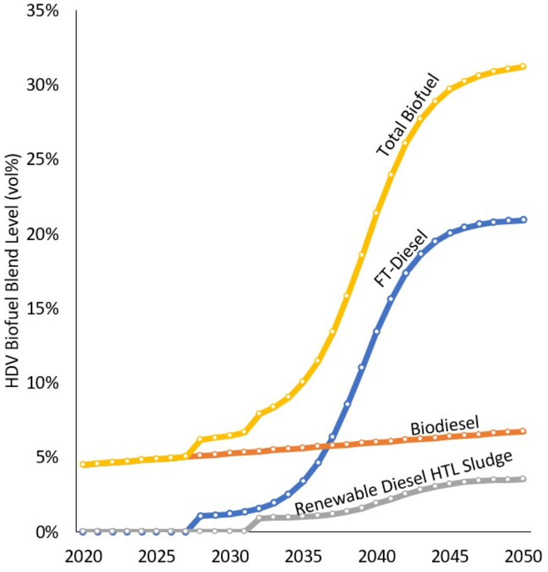
OUTCOMES

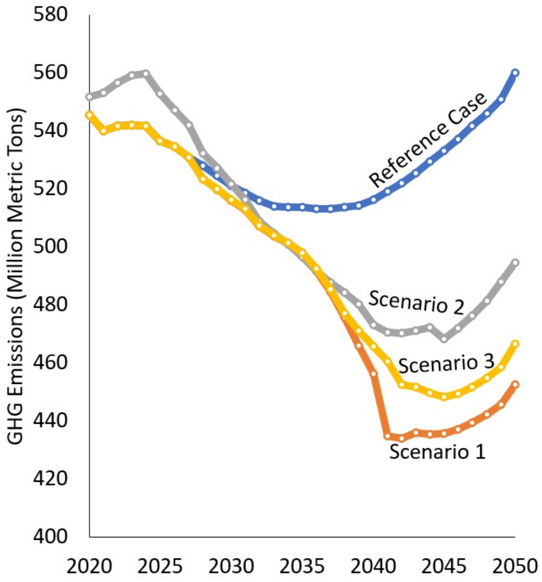
Allocating biomass resources to decarbonize transportation

Potential Biofuel Supply for Heavy-Duty Sector

(Scenario 1)

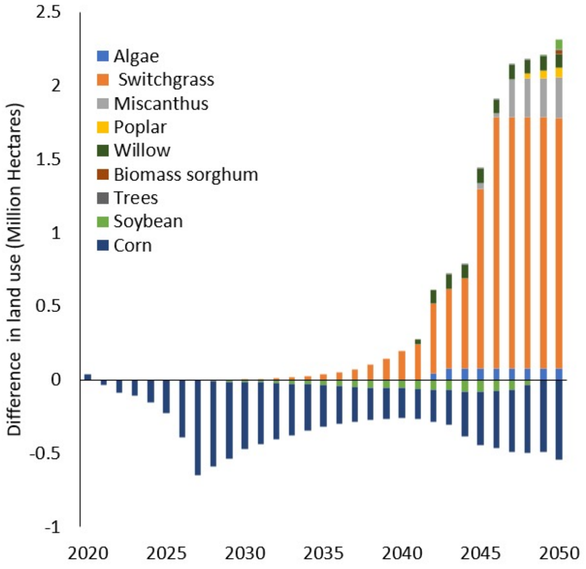


Life Cycle GHG Emissions



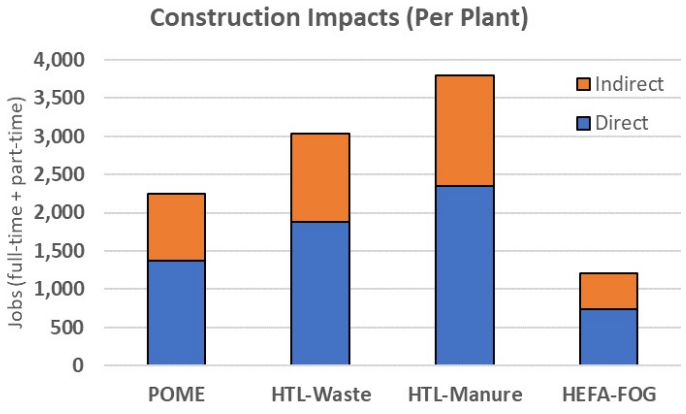
Land Use Change

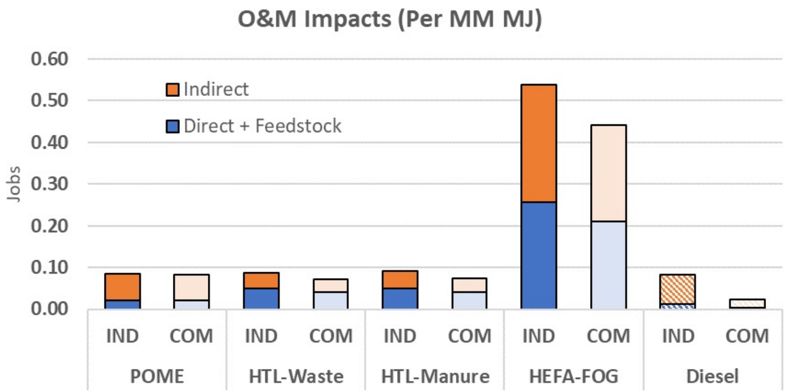
(Scenario 1)



OUTCOMES Biofuel production provides jobs

- Employment for biofuel production is on par with conventional fuels.
  - Shift from petroleum fuels to biofuels would not cause net job loss.
- Construction jobs associated with biofuel infrastructure could be significant, although temporary.



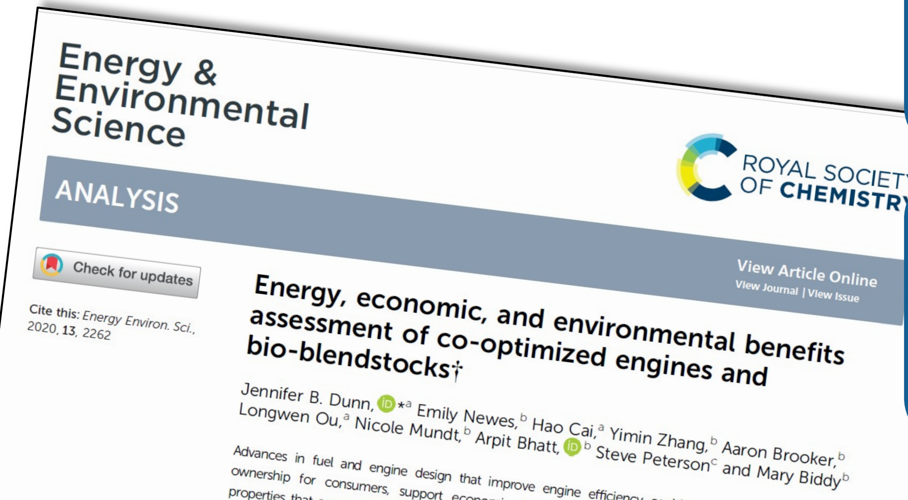


Next Steps

Decarbonizing transportation and ending NO_x and PM emissions at an acceptable cost

NEXT STEPS Integrated analysis for MD/HD vehicles

…analyzes the potential for scale up of Co-Optima vehicles and fuels and potential benefits and tradeoffs.



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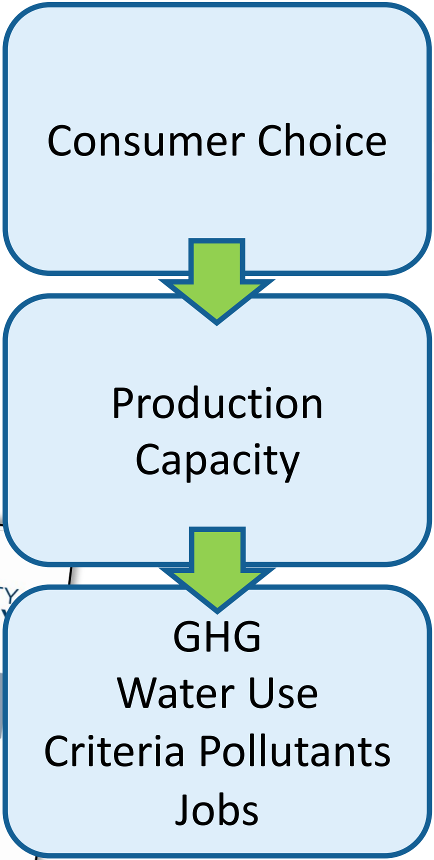
Energy, economic, and environmental benefits assessment of co-optimized engines and bio-blendstocks†

Jennifer B. Dunn,*[a] Emily Newes,[b] Hao Cai,[a] Yimin Zhang,[b] Aaron Brooker,[b] Longwen Ou,[a] Nicole Mundt,[b] Arpit Bhatt,[b] Steve Peterson[c] and Mary Biddy[b]

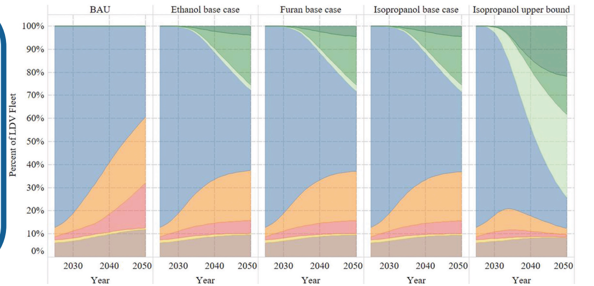
Advances in fuel and engine design that improve engine efficiency
ownership for consumers, support
properties that

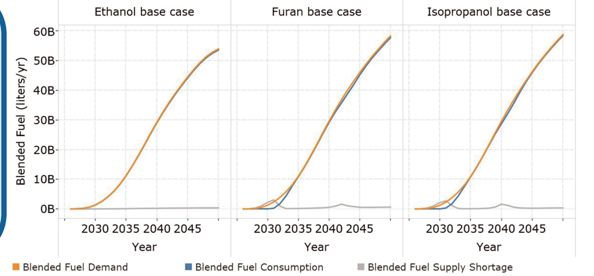


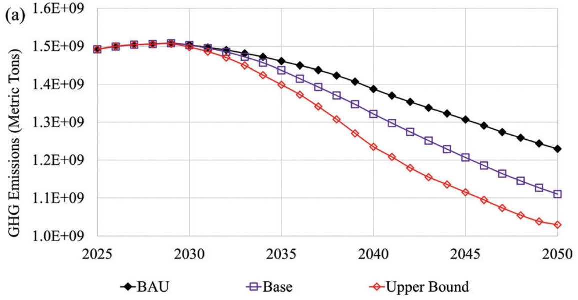
Consumer Choice

Production Capacity

GHG
Water Use
Criteria Pollutants
Jobs







NEXT STEPS Realizing the potential

- Further reduce carbon intensity
- Increase blend level
- Requirements to achieve net-zero criteria pollutants
- Leveraging existing production and distribution infrastructure

Sustainable fuels

Leverage Co-Optima work, further reducing GHG emissions

Expand scope to include e-fuel candidates

Net-zero emissions

Develop engine technologies for soot-less operation

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

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Fuel Technologies

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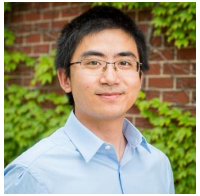
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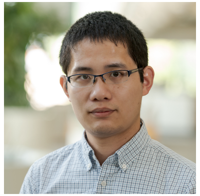
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Steve Phillips


Magdelena Ramirez Corredores


Avantika Singh


Lauren Sittler


Scott Sluder


Mike Talmadge


Ling Tao


Ram Vijayagopal


Yimin Zhang


Greg Zaimes

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

Capstone webinar series – stay tuned

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

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

APR 29

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

Bob McCormick
National Renewable Energy Laboratory

Charles Mueller
Sandia National Laboratories

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

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

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

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Q & A

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