

# DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

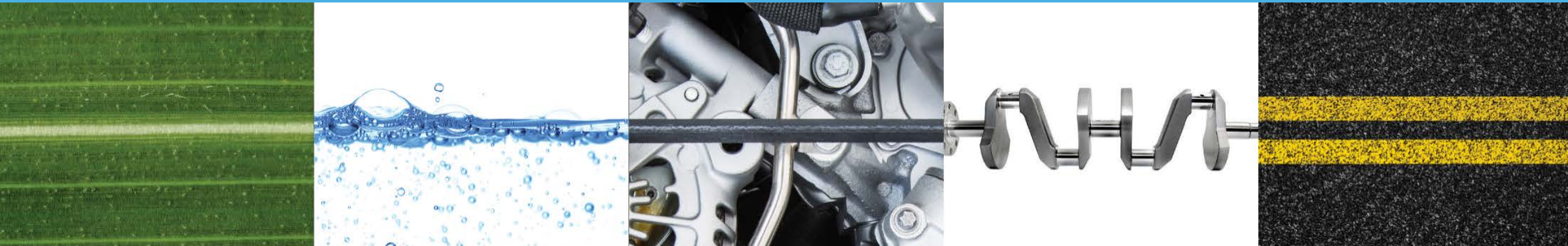
## Co-Optima Program: Potential Impact at Scale

Avantika Singh  
National Renewable Energy Laboratory  
(on behalf of the Analysis Team)  
March 15, 2021



CO-OPTIMIZATION OF  
**FUELS & ENGINES**

better fuels | better vehicles | sooner



# Project Overview

What we do within Co-Optima for impact and refinery integration analysis



## Goal

Estimate the potential benefits of Co-Optima technologies if adopted at scale

## Approach

Deploy state-of-the-art integrated modeling tools using informed inputs from Co-Optima research

## Relevance

Addresses BETO Goals to:

1. Quantify economy-wide benefits from the deployment of Co-optimized fuels/engines in the light- and heavy- duty sectors
2. Identify value of performance advantaged biofuels to the refiners
3. Measure environmental and socio-economic benefits to the community

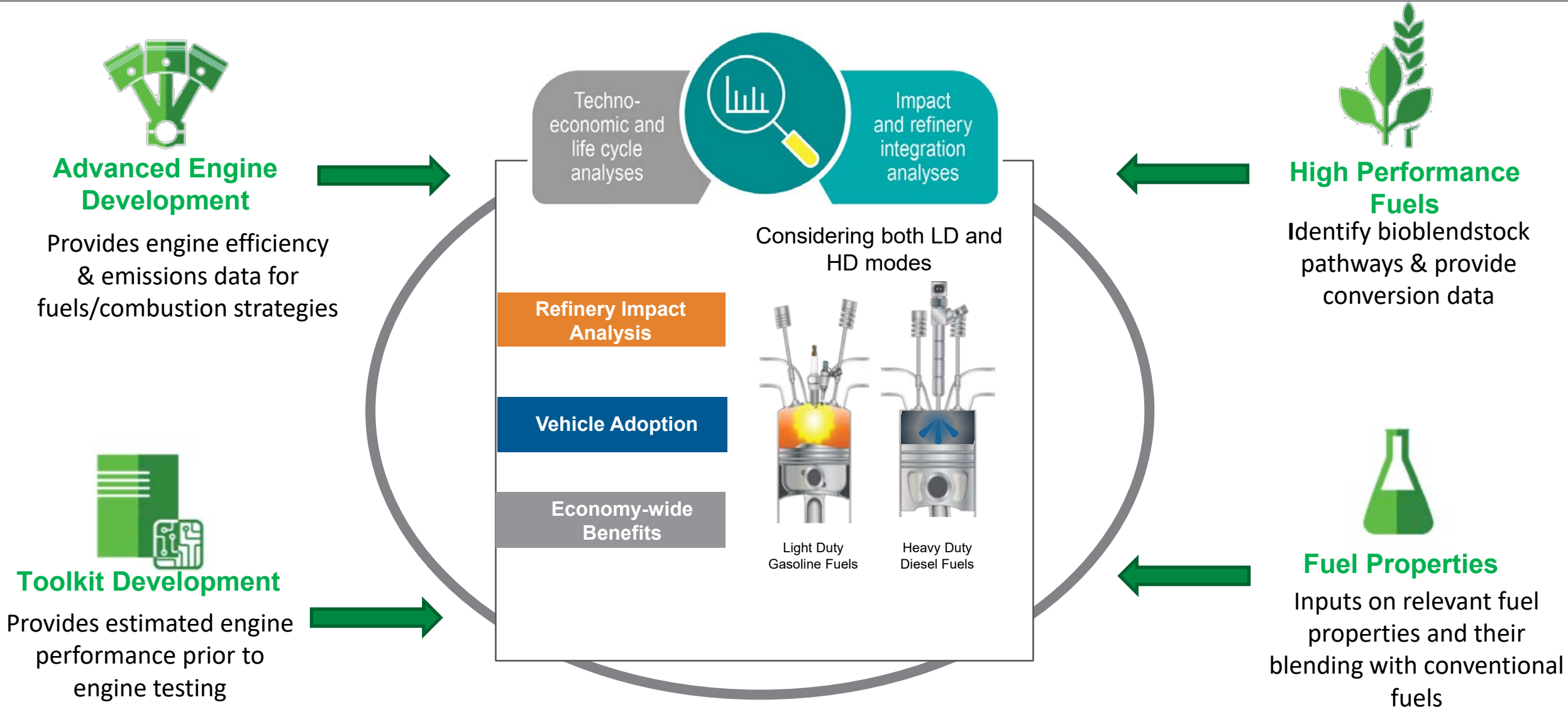


# 1- Management



# 1. Management

Analysis team interacts with every Co-Optima team and guidance from leadership team



Analysis team estimates economic and sustainability implications



# 1. Management

Analysis experts representing core capabilities from different national labs



Troy  
Hawkins  
(Lead)



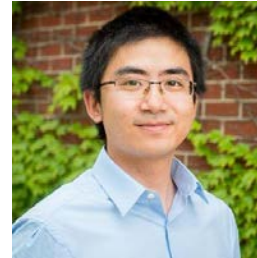
Avantika  
Singh  
(Deputy Lead)



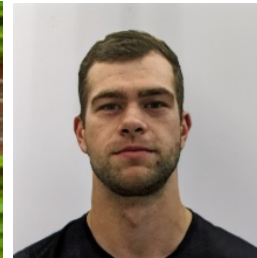
Andre  
Avelino



Aaron  
Brooker



Hao  
Cai



Nick  
Carlson



Scott  
Curran



Jennifer  
Dunn



Yuan  
Jiang



Shuyun  
Li



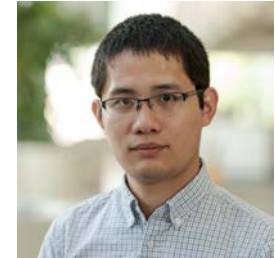
Doug  
Longman



Emily  
Newes



Doris  
Oke



Longwen  
Ou



Lauren  
Sittler



Scott  
Sluder



Mike  
Talmadge



Magdalena  
Ramirez



Ram  
Vijayagopal



Yimin  
Zhang



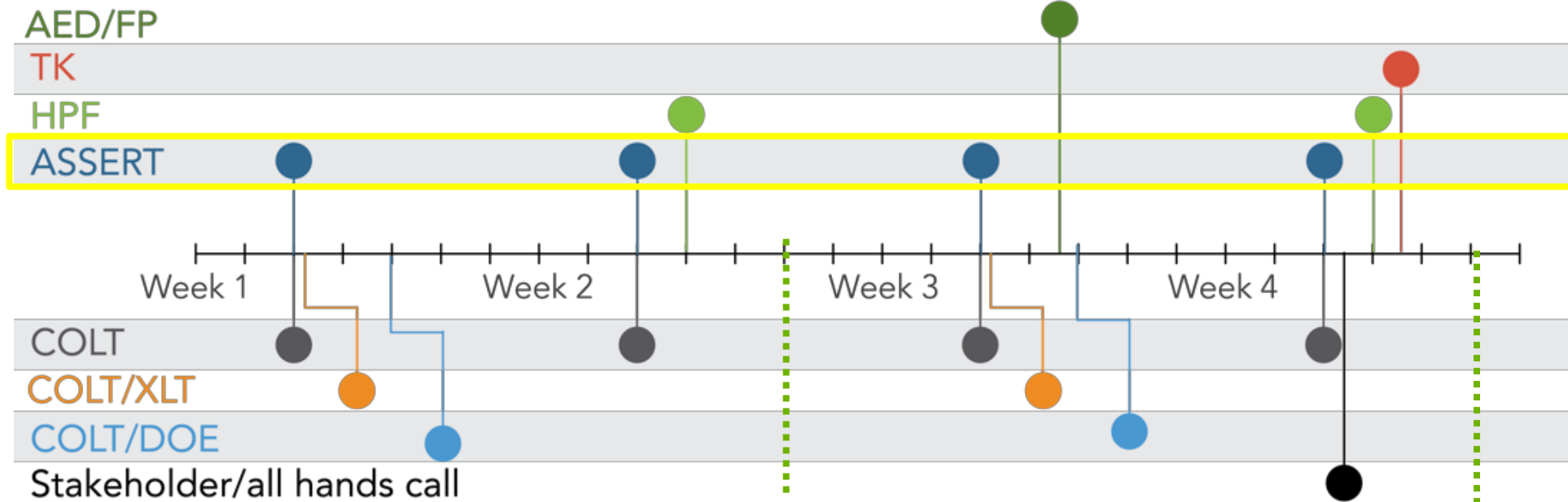
Greg  
Zaimes

# 1. Management

Coordination, Collaboration, and Communication



## Co-Optima regularly scheduled meetings



External Stakeholders

- Quarterly External Advisory Board Meetings*
- Conference Presentations and Posters*
- Upcoming Co-Optima Capstone Webinars*

*Coordination & update meeting between analysis tasks*

*Monthly updates to Co-Optima teams and stakeholders*

# 1. Management

Data availability and delays in data/results handoffs are risks for the analysis team



## Analysis Major Risk Factors



Lack of complete bioblendstock properties or their blending data with conventional fuels at the time of measurements



Work with fuel properties **Co-Optima Fuel Property** team for additional measurements or perform estimates using process modeling tools



Delays or disruption in the timeline for data flow, such as engine efficiency tests, which inform vehicle adoption models



Engage **Advanced Engine Development** team and **industry partners** to explore a range of key parameters and perform sensitivity analysis

Critical path managed closely with internal and external milestones

# 2- Approach



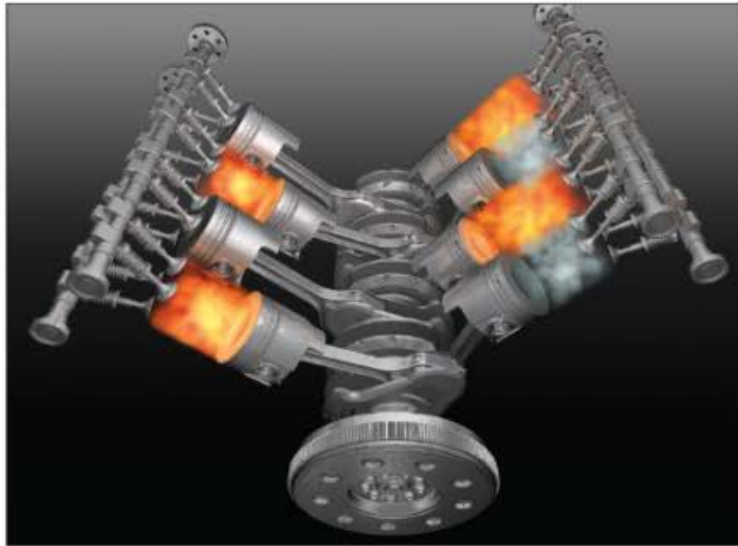


## 2. Approach

Foundational technical questions frame approach



What fuels do  
engines  
*really* want?



What fuel  
options work  
best?



What will work  
in the real world?



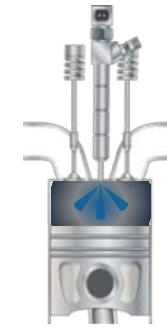
# 2. Approach

Integrated modeling tools for measuring potential impact of light- and heavy-duty modes



**Light Duty**  
RON / MON / S  
Energy Density  
Flash / Boil / Freeze  
RVP / HOV  
Sooting

## Light-Duty and Heavy-Duty Fuels and Combustion Modes



**Heavy Duty**  
Cetane  
Energy Density  
Flash / Boil / Freeze  
Water Sol  
Sooting



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



**Vehicle Adoption**  
How would Co-Optima fuels and vehicles technology penetrate the market?



**Economy-wide Benefits**  
Any socio-economic benefits of Co-Optima fuels/vehicle adoption?

# 2. Approach: Refinery Impact Analysis

Quantifies potential bio-blendstock value to refiners using linear programming tools



## Techno-Economic Analysis

Quantifies production cost for bio-blendstocks

## Refinery Impact Analysis

Quantifies bio-blendstock value to refiners

### Refinery Benefits

What is the value of Co-Optima bio-blendstocks to the refining industry?

Benchmarking against a business-as-usual case, quantify the

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

**Relevance:** Identify fuel properties that would generate **market pull from refiners**, and their **cost and sustainability implications**.

# 2. Approach: Refinery Impact Analysis

Evaluate impact of blending Co-Optima bio-blendstocks to produce finished products



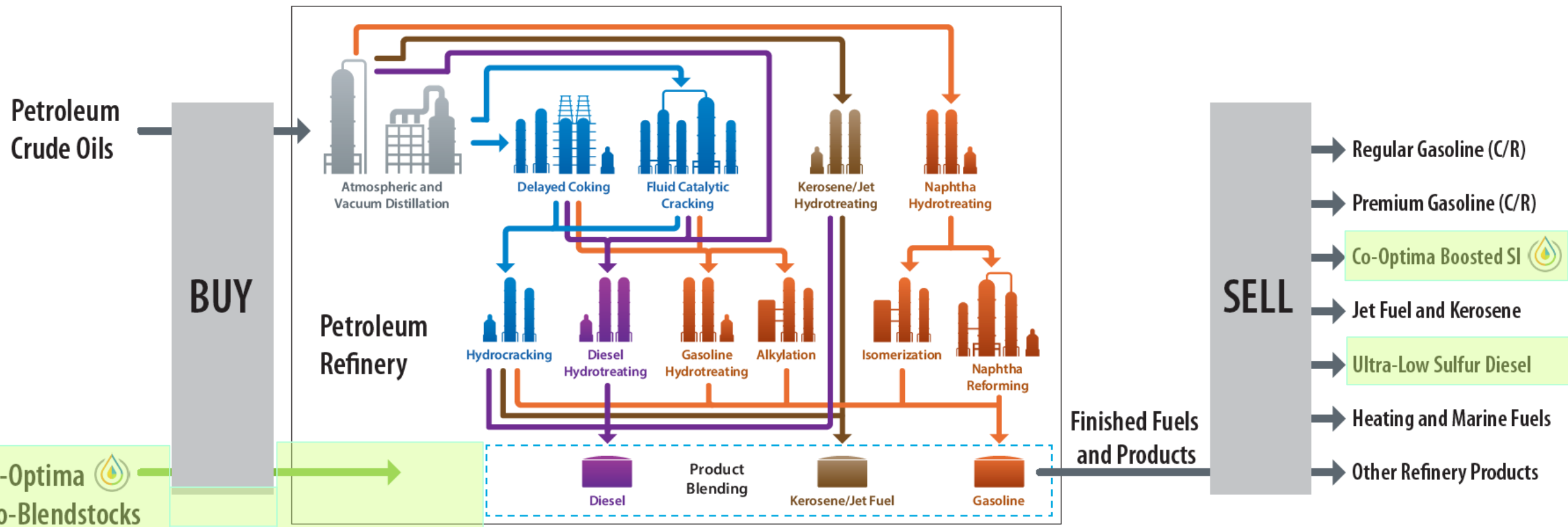
## Overview of Commercial Refinery Modeling Scope in Aspen PIMS

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





# 2. Approach: Refinery Impact Analysis

Co-Optima scenario basis are market relevant that inform the linear programming tools



Refinery configuration and unit capacity basis from EIA.



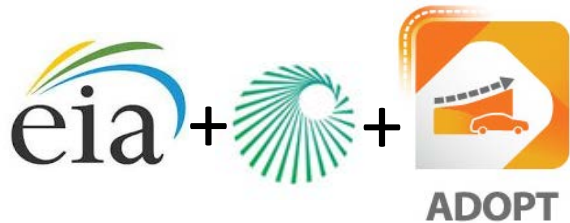
Bio-blendstock costs and blending properties from ASSERT and FP.



ASTM finished fuel specifications are consistent with industry.

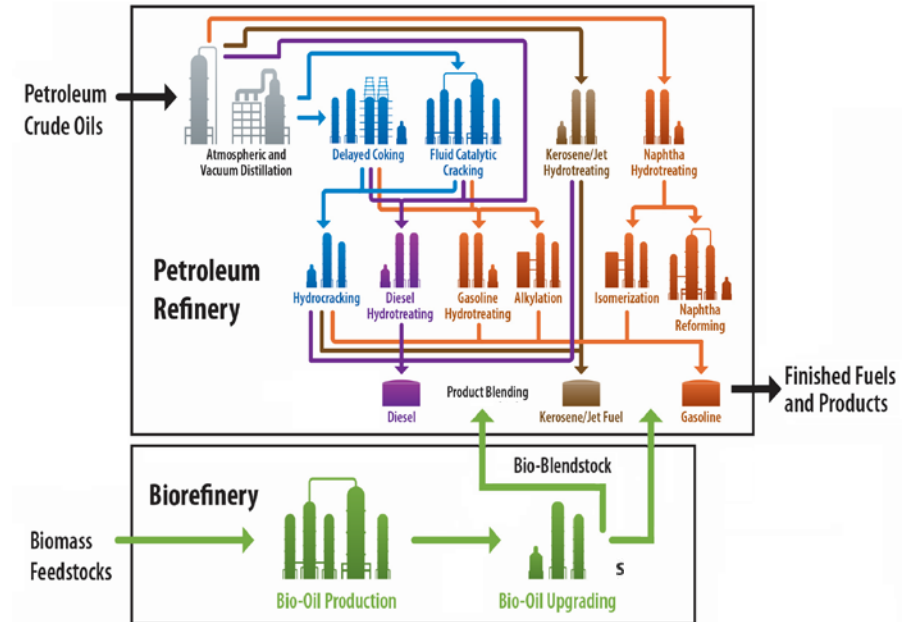


Crude and product pricing data from OPIS by IHS Market.



Fuel market projections from EIA, OPIS, and ADOPT.

## Optimizable Refinery Models



Life Cycle Analysis

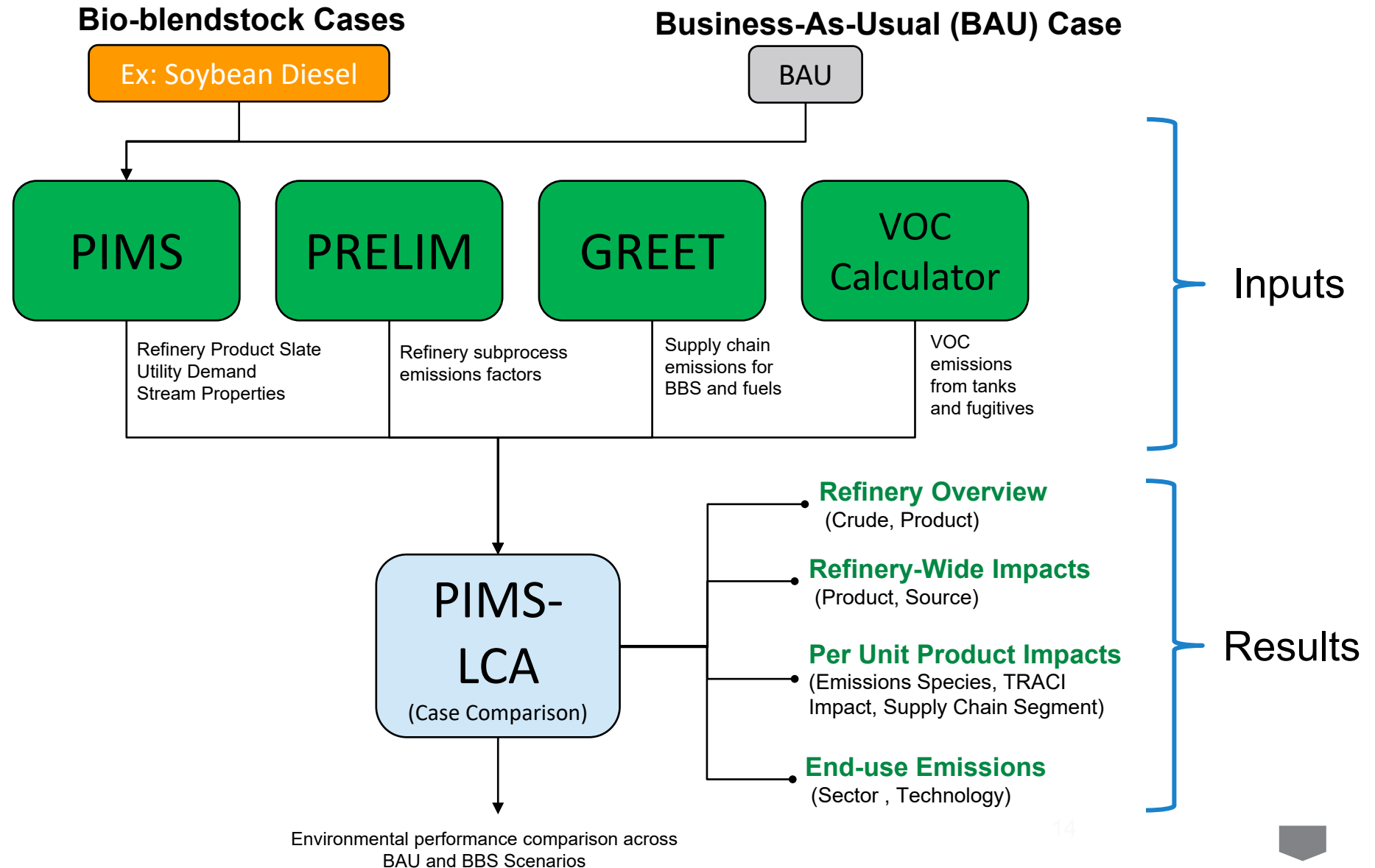


# 2. Approach: Refinery Impact Analysis

Developed LCA tool coupled with refinery models to measure environmental benefits



Excel based tool to inform carbon intensity of refinery emissions



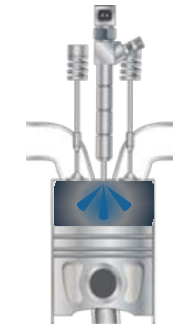
# 2. Approach

Integrated modeling tools for measuring potential impact of light and heavy-duty modes



**Light Duty**  
RON / MON / S  
Energy Density  
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RVP / HOV  
Sooting

## Light-Duty and Heavy-Duty Fuels and Combustion Modes



**Heavy Duty**  
Cetane  
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Sooting



### Refinery Benefits

What is the value of Co-Optima bioblendstocks to the refining industry?



### Vehicle Adoption

How would Co-Optima fuels and vehicles technology penetrate the market?



### Economy-wide Benefits

Any socio-economic benefits of Co-Optima fuels/vehicle adoption?

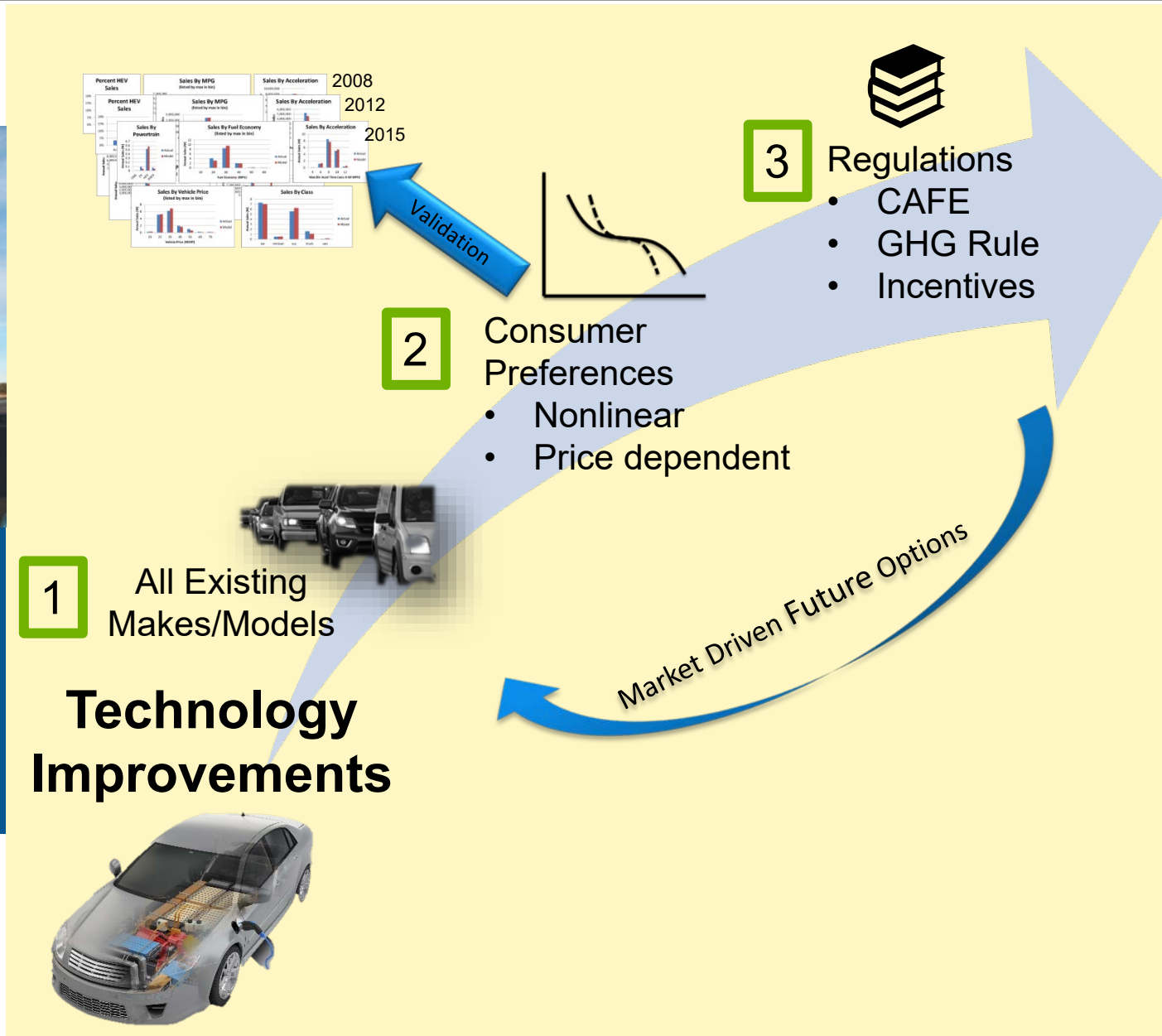
# 2. Approach: Vehicle Adoption

Market factors considered in evolution of Co-Optima vehicles in the automobile fleet

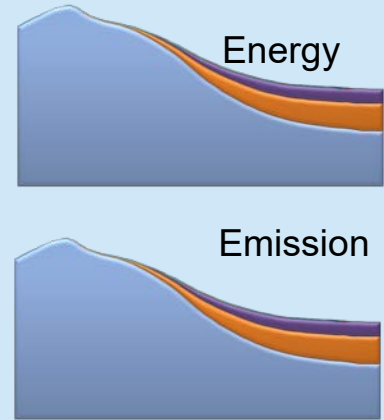


## Vehicle Adoption

How would the Co-Optima fuels and vehicles technology penetrate the market?



## Benefits



Benefits offered by Co-Optima technology<sub>6</sub>



# 2. Approach

Integrated modeling tools for measuring potential impact of light and heavy-duty modes



**Light Duty (LD)**  
RON / MON / S  
Energy Density  
Flash / Boil / Freeze  
RVP / HOV  
Sooting

## Light-Duty and Heavy-Duty Fuels and Combustion Modes



**Heavy Duty (HD)**  
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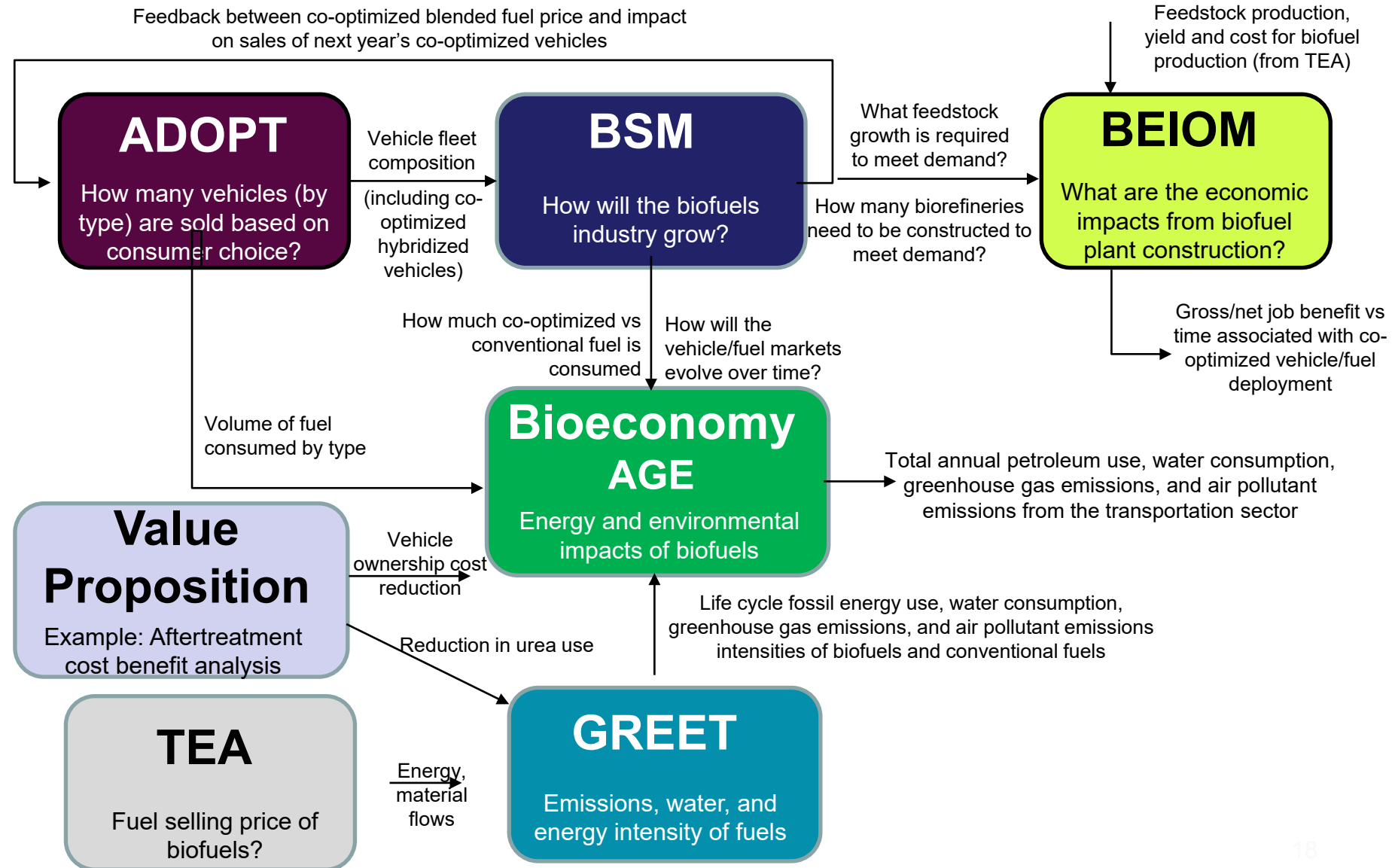
# 2. Approach: Economy-wide Benefits

Integrated benefits analysis framework for measuring sector-wide impacts



## Economy-wide Benefits

Any socio-economic benefits of Co-Optima fuels/vehicle adoption?



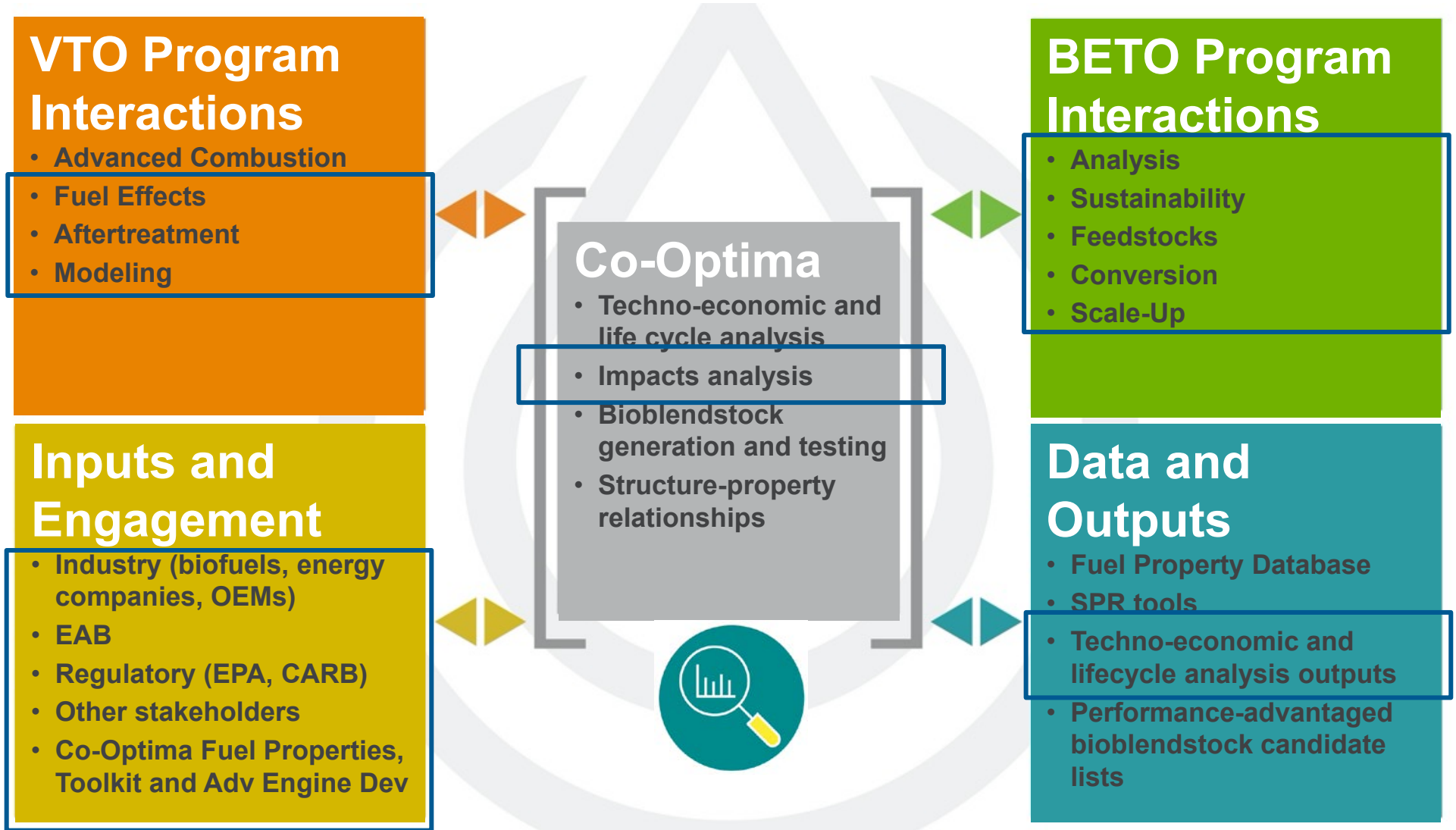


# 3- Impact



# 3. Impact

Co-Optima connects with stakeholders, and the broader BETO and VTO programs



# 3. Impact

Leveraging and interacting with other BETO efforts and disseminates results



## Furthering BETO Goals

Advance public knowledge by sharing state of technology, identifying opportunities & barriers for biofuels scaleup/adoption



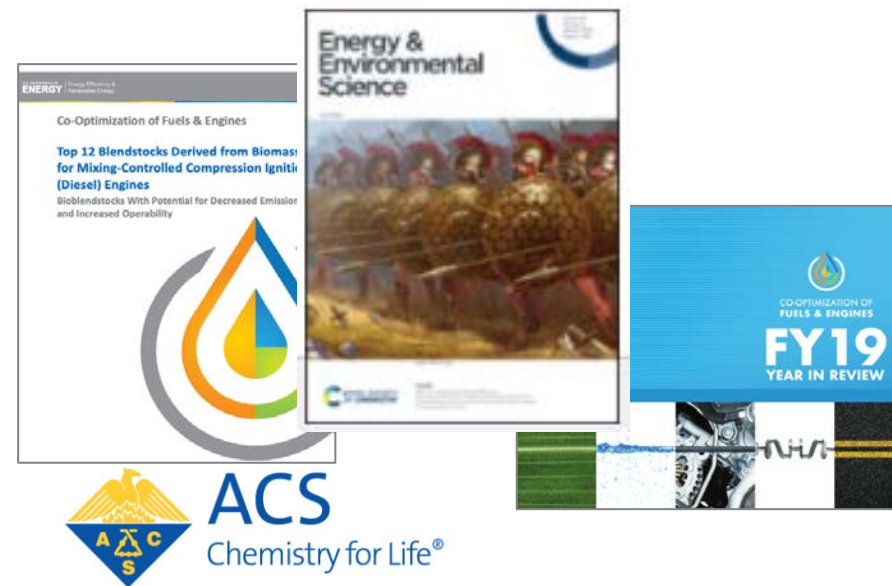
Inform BETO program of promising bioblendstocks from refiners' perspective for gasoline, diesel, jet, and marine fuels, including co-processing strategies



Insights from system-wide modeling (including feedstock assessments) inform potential socio-economic benefits of advancing the bioeconomy



## Engagements & Disseminating Results



Inform public and key stakeholders in peer-reviewed journals, Co-Optima reports, public databases, conferences, and industry engagements, such as interactions with American Petroleum Institute, Environmental Protection Agency, National Biodiesel Board, etc.

# 3. Impact

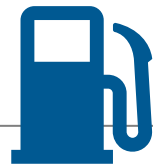
Share insights for a Sustainable Transportation Strategy



## Outcome & Impact

**Outcome:** Information on scalability, economic viability, and environmental/socio-economic benefits of low carbon bioblendstocks

**Impact:** Estimated potential impact of Co-Optima technology adoption at scale, with demonstrated **engine efficiency improvements, emission reductions, & domestic job growth**



## Stakeholder Engagement

- ✓ Attend Co-Optima quarterly **External Advisory Board** meetings
- ✓ Share results and receive feedback from **leadership team** and the **Board of Directors**
- ✓ Present research findings at the monthly **Co-Optima stakeholder** calls



## Disseminating Results

- ✓ Journal Articles (3 published, 9 in preparation) and several conference presentations
- ✓ Annual Co-Optima Year in Review and other reports collating major findings
- ✓ Co-Optima Capstone webinars scheduled on LD and HD sector benefits



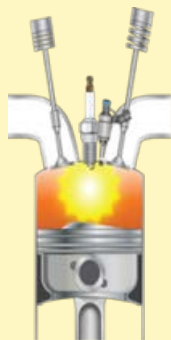
# 4- Progress and Outcomes





# 4. Progress and Outcomes: Light Duty Sector

Integrated modeling tools for measuring potential impact of light- and heavy-duty modes



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RON / MON / S  
Energy Density  
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## Light-Duty and Heavy-Duty Fuels and Combustion Modes



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### Refinery Benefits

What is the value of Co-Optima bioblendstocks to the refining industry?



### Vehicle Adoption

How would Co-Optima fuels and vehicles technology penetrate the market?

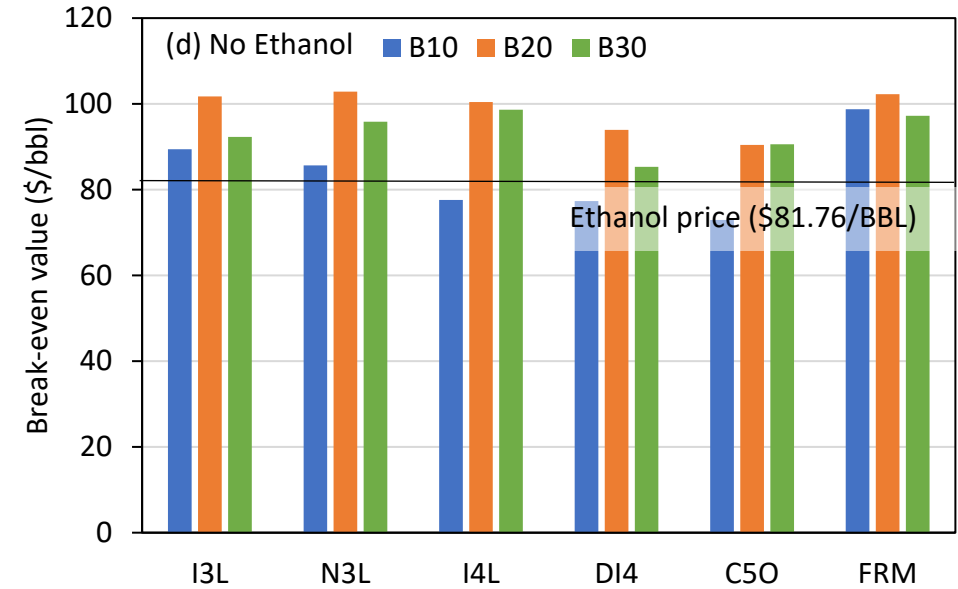
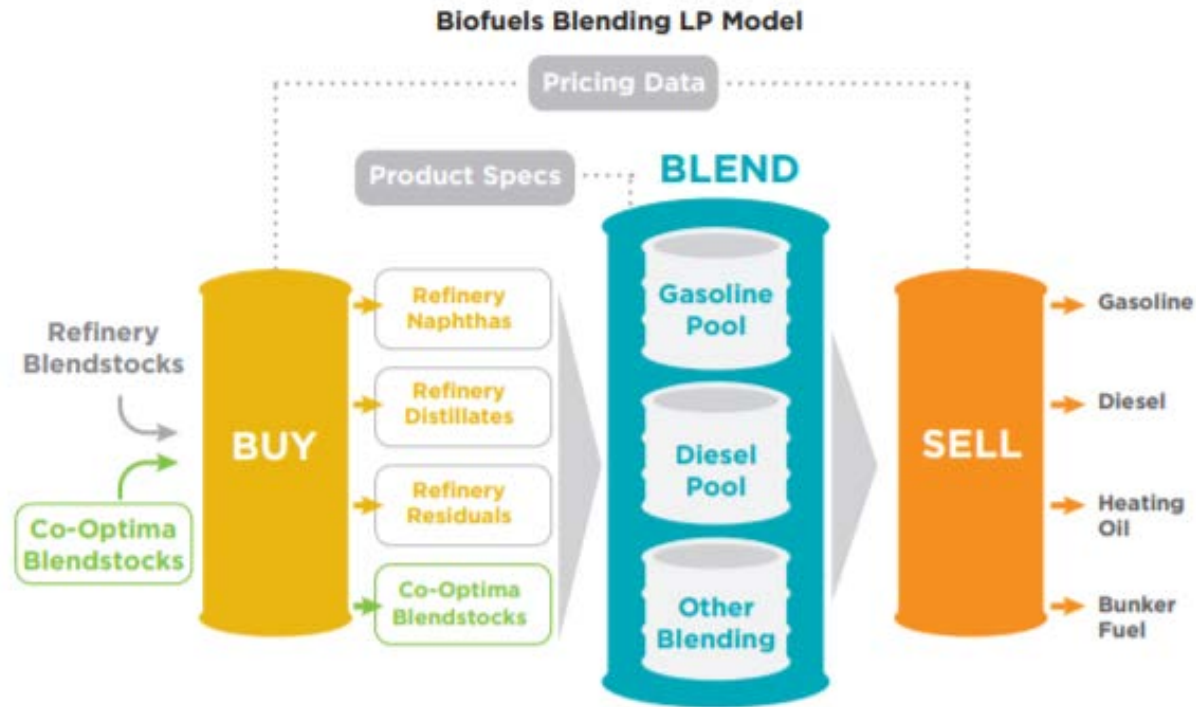


### Economy-wide Benefits

Any socio-economic benefits of Co-Optima fuels/vehicle adoption?

# 4. Progress and Outcomes: Refinery Impacts (LD)

Blending optimization estimated economic value of Co-Optima bioblendstocks



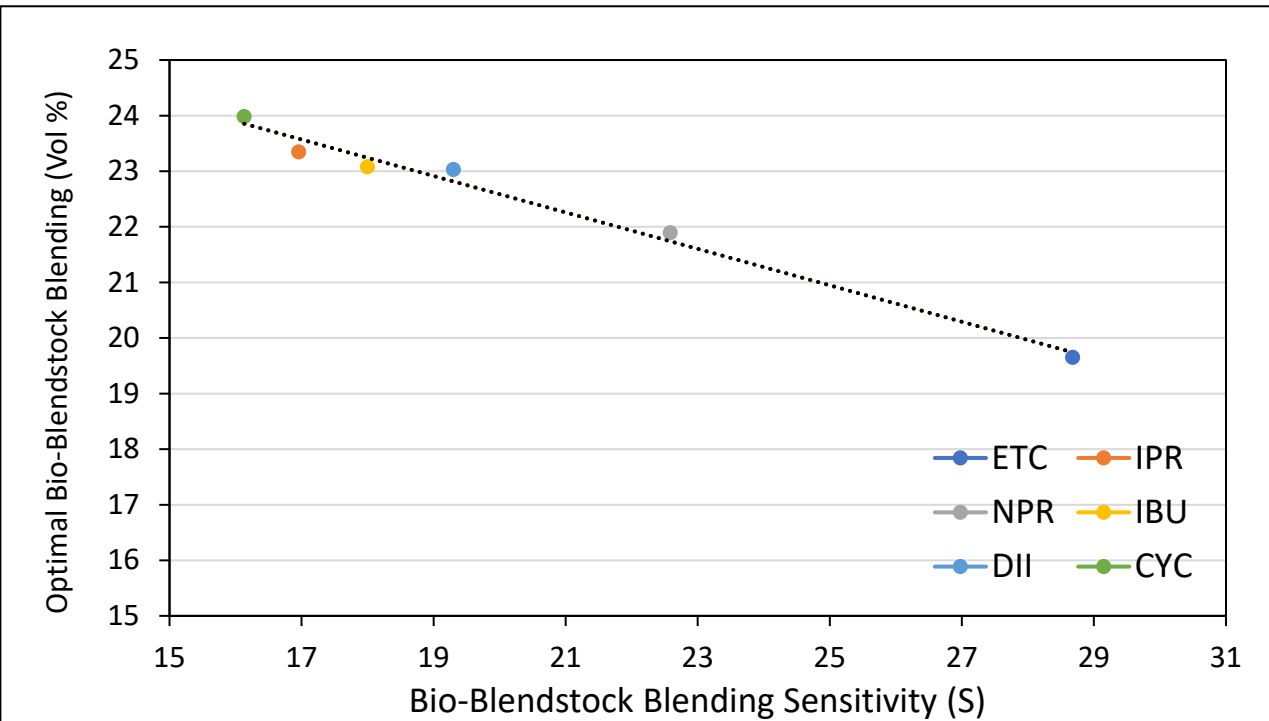
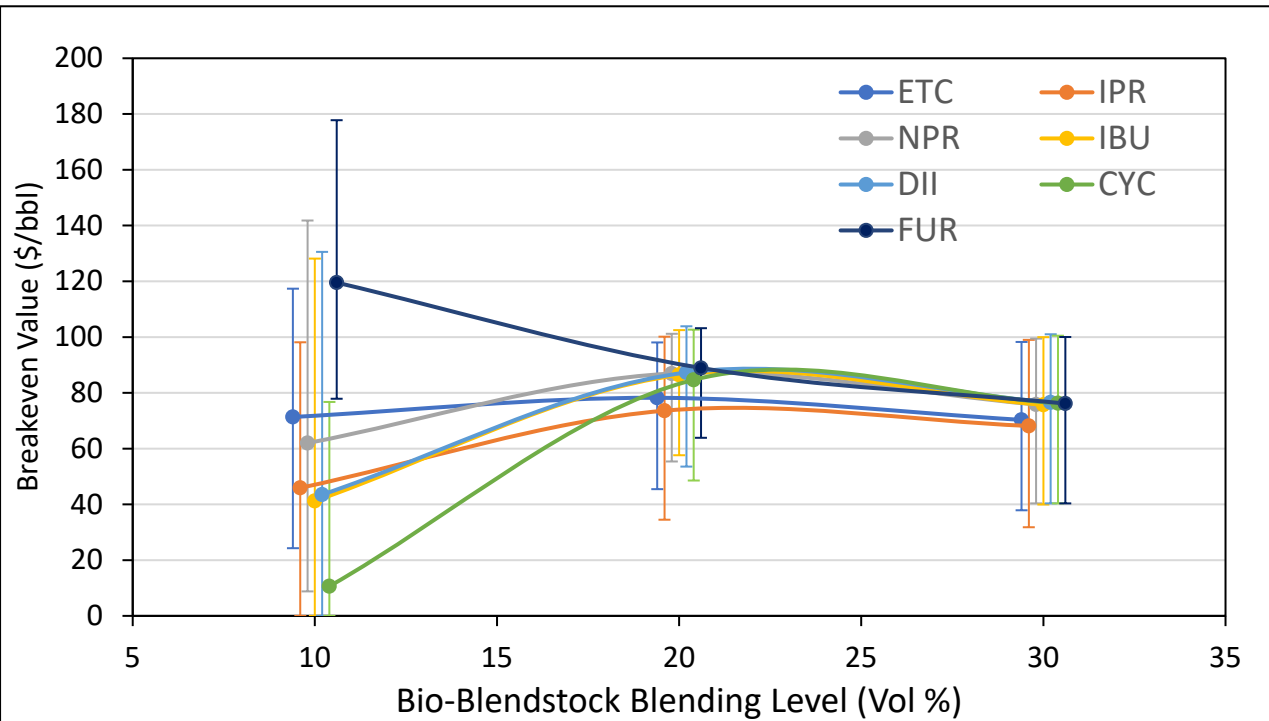
I3L=i-propanol; N3L=n-propanol; I4L=i-butanol;  
DI4=diisobutylene; C5O=cyclopentanone; FRM=furans mix

## Key Outcome:

Co-Optima selected **gasoline-range bioblendstocks (high RON, low RVP)** demonstrate similar advantages as ethanol and can be combined with different refinery naphtha streams to produce **premium gasoline**

# 4. Progress and Outcomes: Refinery Impacts (LD)

Fuel characteristics (RON and S) of Co-Optima biofuels drive economic benefits to refiners



ETC= ethanol; IPR=i-propanol; NPR=n-propanol; IBU=i-butanol; DII=diisobutylene; CYC=cyclopentanone; FUR=furans mix

## Key Outcomes:

(1) Potential value of bio-blendstocks to refiners depends on the **fuel characteristics (RON and S)** and **varies with biofuel blending levels**

(2) Optimal blending ratio that maximized profitability for each bio-blendstock strongly correlated with the **fuel sensitivity**



# 4. Progress and Outcomes: Vehicle Adoption (LD)

Vehicle choice model predicts penetration of Co-Optima engines in the market

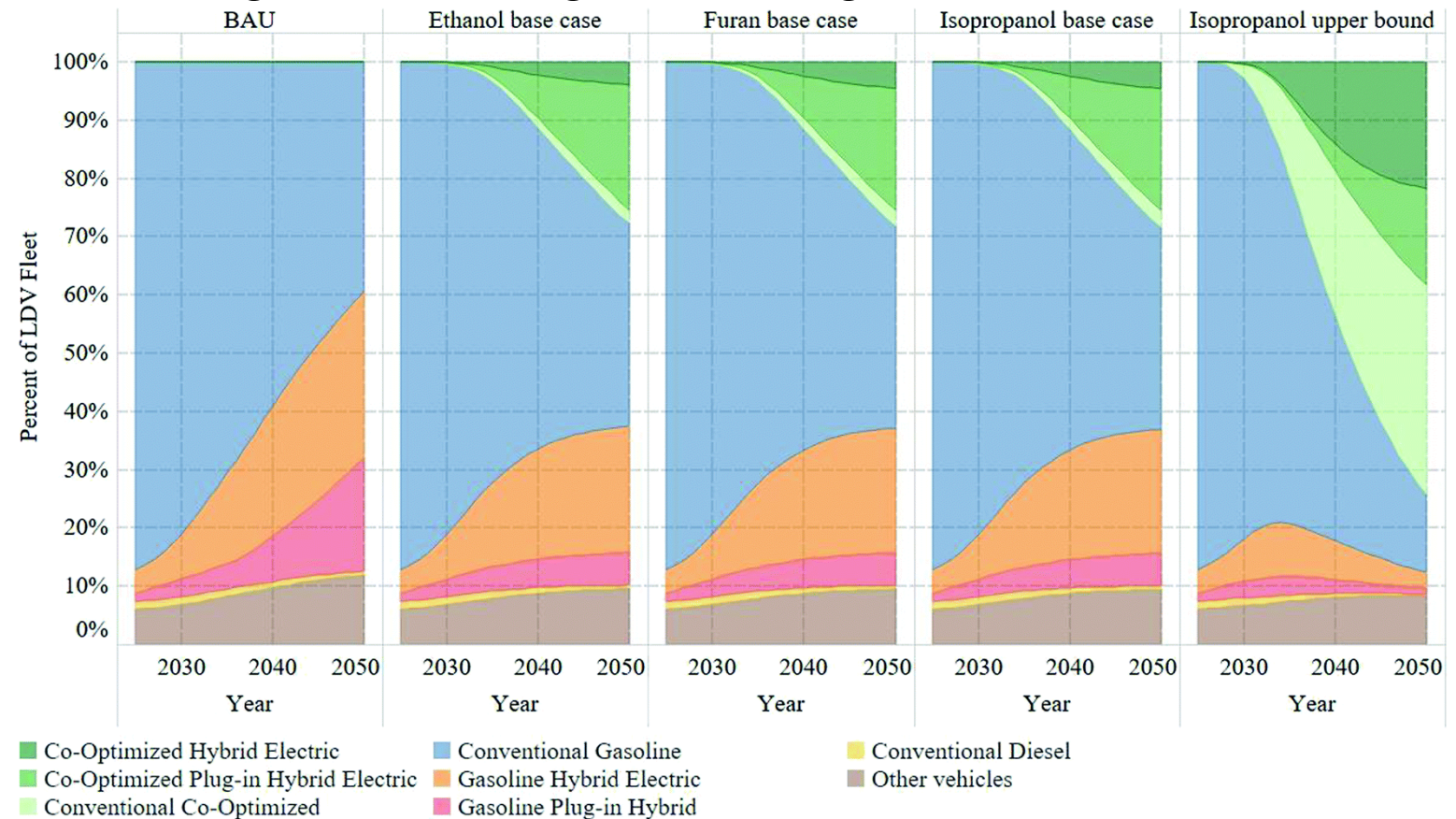


## Vehicle Adoption

How would the Co-Optima fuels and vehicles technology penetrate the market?

### Key Outcome:

Co-optimized vehicles become the best-selling vehicle after 2035 because they combine - **better performance** and - **lower fuel cost per mile** compared to the best-selling conventional gasoline and gasoline PHEV vehicles.



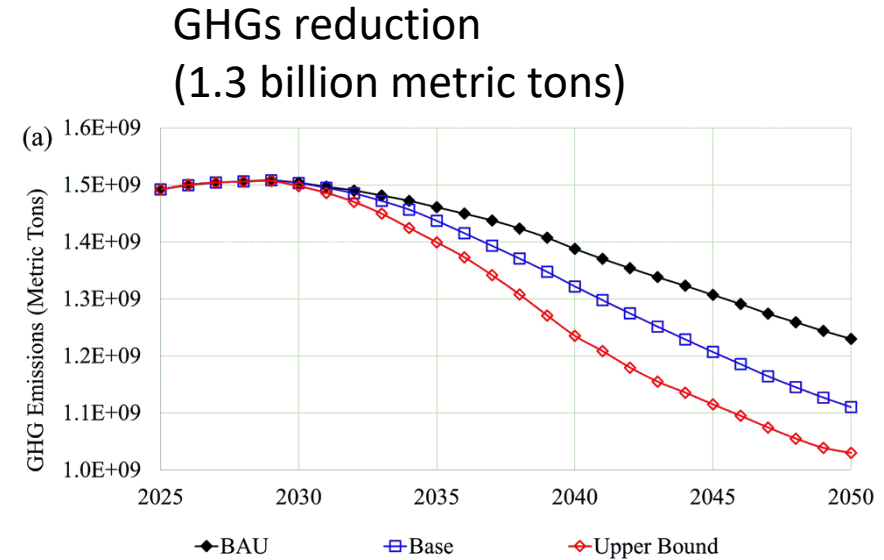
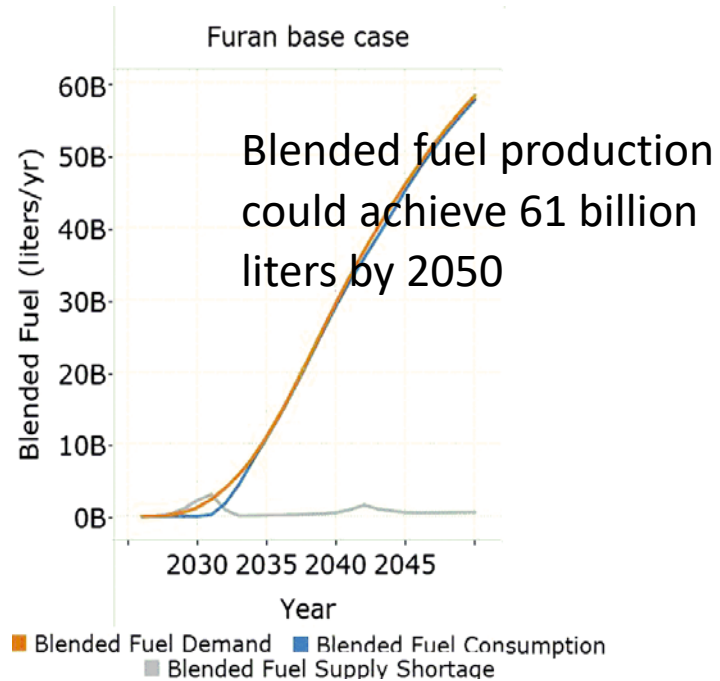
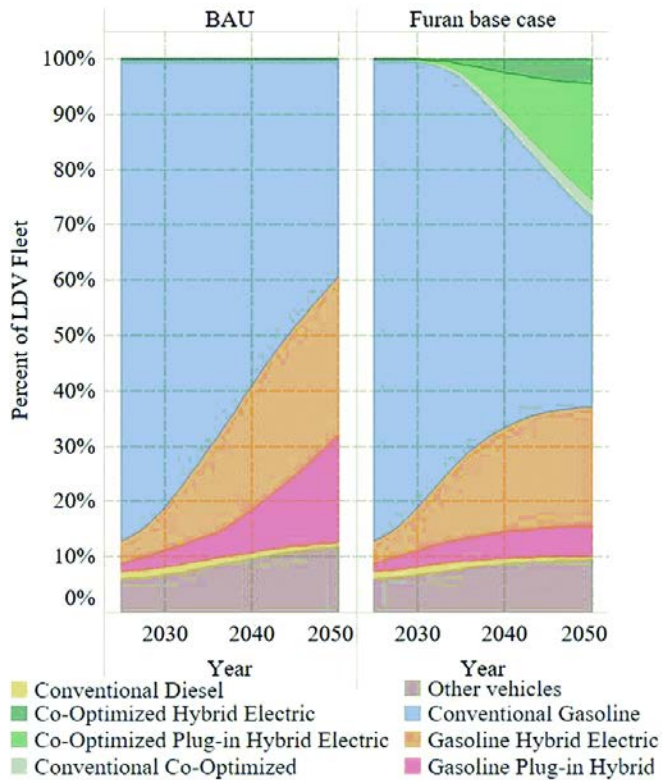


# 4. Progress and Outcomes: Economy-wide Benefits (LD)



Co-Optimized fuels and vehicle technology lead to significant emissions reductions

## Key Outcomes:



### Vehicle Adoption

Co-optima fuels/engines could achieve 10% efficiency gains compared to E10

### Biofuels Production, Jobs

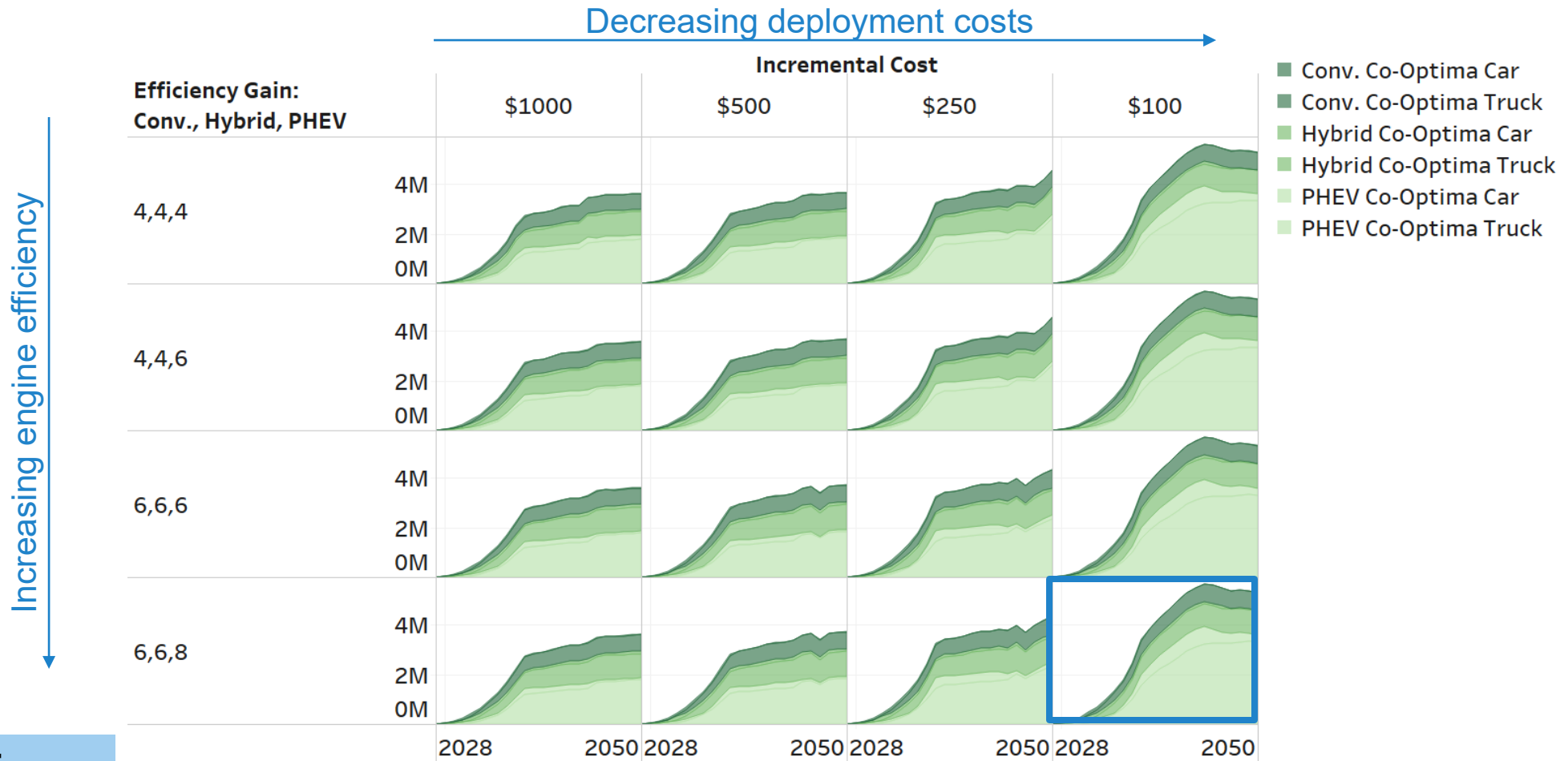
Diversifying the fuel resource base leads to significant job creation, esp. in rural areas

### Reduction in GHGs, Criteria Pollutants

Significant reductions in GHG and PM2.5 over 2025-2050

# 4. Progress and Outcomes: Vehicle Adoption (LD)

Vehicles with hybridized power trains could experience a synergistic efficiency increase



## Key Question:

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

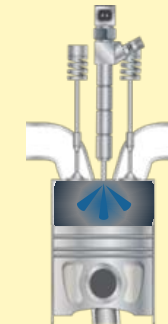
# 4. Progress and Outcomes: Heavy Duty Sector

Integrated modeling tools for measuring potential impact of light- and heavy-duty modes



**Light Duty**  
RON / MON / S  
Energy Density  
Flash / Boil / Freeze  
RVP / HOV  
Sooting

## Light-Duty and Heavy-Duty Fuels and Combustion Modes



**Heavy Duty**  
Cetane  
Energy Density  
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Water Sol  
Sooting



### Refinery Benefits

What is the value of Co-Optima bioblendstocks to the refining industry?



### Vehicle Adoption

How would Co-Optima fuels and vehicles technology penetrate the market?



### Economy-wide Benefits

Any socio-economic benefits of Co-Optima fuels/vehicle adoption?

# 4. Progress and Outcomes: Vehicle Adoption (HD)

Understanding the heavy-duty value proposition – reduced aftertreatment costs



ENVIRONMENTAL  
Science & Technology

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pubs.acs.org/est

## Co-optimization of Heavy-Duty Fuels and Engines: Cost Benefit Analysis and Implications

Longwen Ou,<sup>1</sup> Hao Cai,<sup>1\*</sup> Hee Je Seong,<sup>2</sup> Douglas E. Longman,<sup>2</sup> Jennifer B. Dunn,<sup>1</sup> John M. E. Storey,<sup>3</sup> Todd J. Toops,<sup>3</sup> Josh A. Pihl,<sup>3</sup> Mary Biddy,<sup>1</sup> and Matthew Thornton<sup>1</sup>

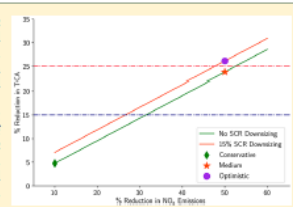
<sup>1</sup>Systems Assessment Center, Energy Systems Division, and <sup>2</sup>Center for Transportation Research, Energy Systems Division, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, Illinois 60439, United States

<sup>3</sup>Fuels, Engines, and Emissions Research Center, Oak Ridge National Laboratory, NTRC Building, 2360 Cherrahala Boulevard, Knoxville, Tennessee 37932, United States

<sup>4</sup>National Bioenergy Center, and <sup>5</sup>Transportation and Hydrogen Systems Center, National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, Colorado 80401, United States

### Supporting Information

**ABSTRACT:** Heavy-duty vehicles require expensive aftertreatment systems for control of emissions such as particulate matter (PM) and nitrogen oxides (NO<sub>x</sub>) to comply with stringent emission standards. Reduced engine-out emissions could potentially alleviate the emission control burden, and thus bring about reductions in the cost associated with aftertreatment systems, which translates into savings in vehicle ownership. This study evaluates potential reductions in manufacturing and operating costs of re-designed emission aftertreatment systems of line-haul heavy-duty diesel vehicles (HDDVs) with reduced engine-out emissions brought about by co-optimized fuel and engine technologies. Three emissions reduction cases representing conservative, medium, and optimistic engine-out emission reduction benefits are analyzed, compared to a reference case: the total costs of aftertreatment systems (TCA) of the three cases are reduced to \$11,400 (1.63 €/km), \$9,100 (1.30 €/km), and \$8,800 (1.26 €/km), respectively, compared to \$12,000 (1.71 €/km) for the reference case. The largest potential reductions result from reduced diesel exhaust fluid (DEF) usage due to lower NO<sub>x</sub> emissions. Downsizing aftertreatment devices is not likely, because the sizes of devices are dependent on not only engine-out emissions, but also other factors such as engine displacement. Sensitivity analysis indicates that the price and usage of DEF have the largest impacts on TCA reduction.



### INTRODUCTION

Emissions of criteria pollutants such as oxides of nitrogen (NO<sub>x</sub>), particulate matter (PM), unburned hydrocarbons (HC), and carbon monoxide (CO) from mixing-controlled compression-ignition (MCCI) (or diesel) engines raise health and air quality concerns. Heavy-duty diesel vehicles (HDDVs) accounted for 43% of NO<sub>x</sub> and 47% of PM emissions from all on-road vehicles in the US in 2014.<sup>1</sup> Emission standards for HDDVs, which began in the late 1980s, have resulted in increasingly stringent limits on pollutant emissions from new HDDVs and have promoted progress in emission control technologies. Since 2010, all domestic HDDVs have been equipped with both in-cylinder emission control strategies such as exhaust gas recirculation (EGR), and a series of aftertreatment devices, which typically include diesel oxidation catalysts (DOC), diesel particulate filters (DPF), and urea selective catalytic reduction (SCR) for NO<sub>x</sub> emissions control. These devices cooperate with each other for improved efficiency of emission control and maximized durability. For instance, DOC

not only oxidizes part of the NO to NO<sub>2</sub>, which is critical for effective operations of DPF and SCR, but also generates heat for active regeneration of DPF by oxidation of injected fuel. Details of these devices are discussed in the Supporting Information (SI). Stringent emission regulations have driven up emission control costs for HDDVs, with aftertreatment systems being the major cost driver.<sup>2</sup>

Both engine operating conditions and fuel properties can affect exhaust emissions.<sup>3</sup> For instance, the effects of fuel properties on NO<sub>x</sub> emissions depend on factors such as (a) how physical properties of a fuel affect its evaporation, mixing processes, and peak combustion temperature; and (b) the effects of fuel properties on the initial fuel-rich flame-ignition event.<sup>4–6</sup> Several diesel fuel properties, including fuel cetane number,

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Environ. Sci. Technol. 2019, 53, 12904–12913

## Key Questions:

What is the potential for adoption of Co-Optima technologies by **Class 8 Heavy-Duty Trucks**?

- Reduced cost of aftertreatment by 5-26% over the lifetime of the vehicle

How do the potential benefits\* from Co-Optima technologies compare with those from other technologies?

- Electrification
- Renewable diesel
- Co-Optima technologies in conjunction

These findings are currently being incorporated into economy-wide benefits analysis

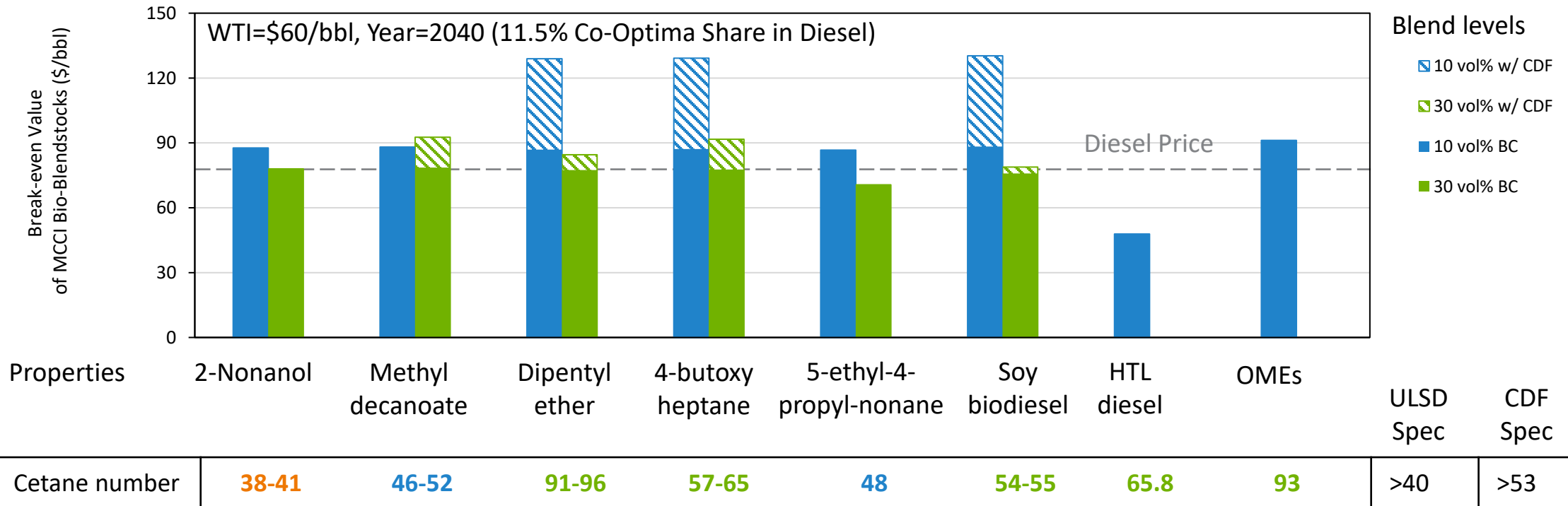
\*Key metrics: GHGs, CAPs, water use, energy use, total cost of ownership, jobs



# 4. Progress and Outcomes: Refinery Impacts (HD)



MCCI bio-blendstocks reduce the extent of hydrotreatment necessary to meet sulfur specs



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

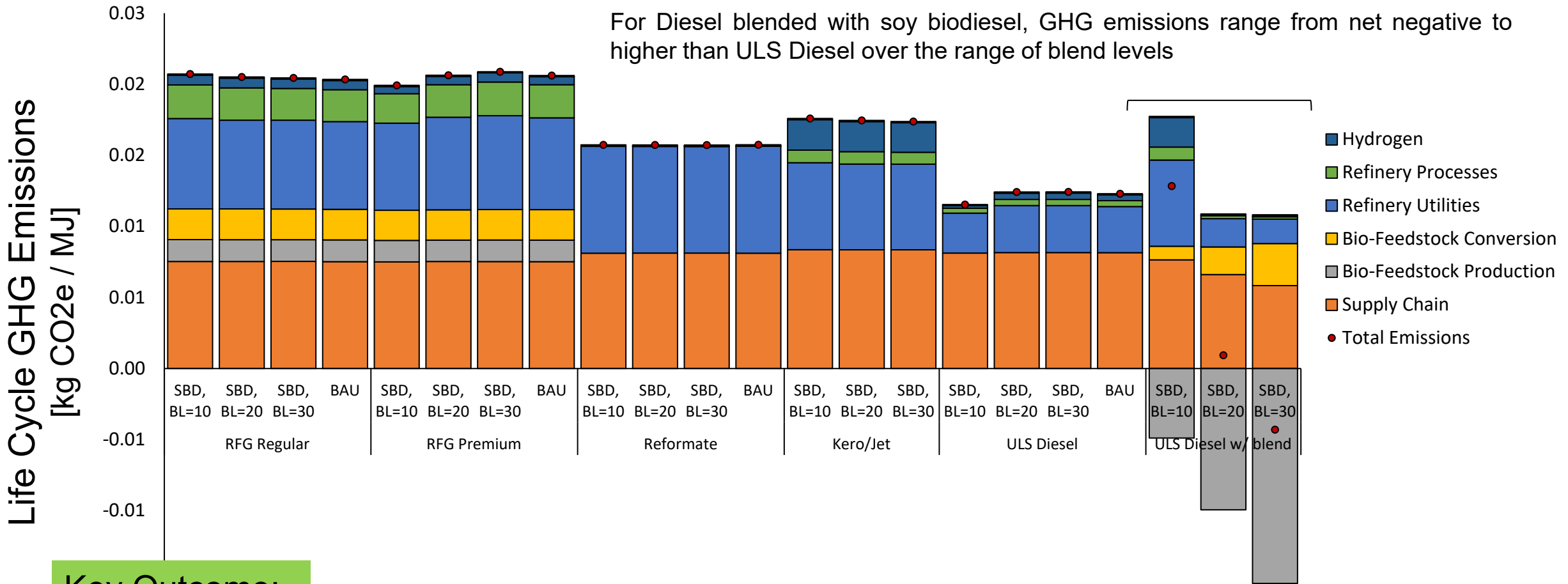
OMEs = oxymethylene ethers, ULSD = ultra-low sulfur diesel, CDF = California diesel fuel, MCCI = Mixing Controlled Compression Ignition, WTI= West Texas Intermediate, BC = base case

## Key Outcomes:

- High-Cetane Number (CN) Bioblendstock will create extra value, if demand for high-CN diesel increases
- BBS properties that help refinery constraints are the most important such as sulfur reduction, followed by CN & density

# 4. Progress and Outcomes: Refinery Impacts (HD)

Significant GHG reduction from cradle-to-refinery gate analysis of Soy Biodiesel



**Key Outcome:**

Biofuel blending levels can have non-linear impacts on the refinery's environmental performance

# Summary





## Light Duty

- 10% fuel economy gain over 2015 baseline

## Medium- and Heavy-Duty

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

## Biofuels

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

## Crosscutting Goals

- Reduce greenhouse gas 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



# Summary



## Overview

Analysis supports Co-Optima's goal to identify low carbon fuel-engine combinations that increase fuel economy and reduce emissions by assessing bioblendstocks across economic, environmental, and scalability metrics. We evaluate refinery impacts of blending Co-Optima bioblendstocks into finished fuels as well as economy-wide environmental and socio-economic benefits of Co-Optima technology adoption.

## Management

- Analysis Tasks are well-organized, tracked by milestones (internal/external), undergo multi-level quality checks.
- Regular interactions with other Co-Optima Teams and coordinate with other BETO analysis efforts.
- Regular meetings with External Advisory Board and stakeholders.
- Disseminate results through articles, reports, and conference presentations.

## Approach

- Identify biofuel fuel properties that would generate market pull from refiners, and their cost and sustainability implications.
- Vehicle adoption models indicate the penetration of co-optimized vehicles, which serves as the basis for integrated analysis informs overall environmental and socio-economic benefits.

## Impact

- Enhance the value proposition for biofuels by identifying scalable, economically viable bioblendstocks that maximize engine performance and energy efficiency and minimize environmental impacts.
- Petroleum consumption, GHG emissions, water consumption, and PM2.5 emissions are all reduced when co-optimized fuels and engines emerge.

## Progress & Outcomes

- Refinery impact analysis indicates that high octane, high sensitivity fuels (BSI and MM bio-blendstocks) and low sulfur, high cetane fuels (MCCI) could be valuable to refiners.
- Coupled LCA model development shows the decrease in refinery emissions and criteria pollutants.
- Efficiency increase with Co-Optima fuels and engine combination is the largest driver for LD adoption and reduction in aftertreatment costs is the key factor for HD adoption.
- Integrated benefits analysis demonstrate better air quality impacts and increase in domestic job growth.

# Quad Chart Overview



## Timeline

- Phase 1: October 1, 2015 to September 30, 2018
- Phase 2: October 1, 2019 to September 30, 2021

	FY20	Active Project
<b>DOE Funding</b>	\$1,700K	\$6,235K

## Partner Labs

- ANL, NREL, PNNL (in coordination with INL, LANL, LBNL, LLNL, ORNL, SNL)

## Barriers addressed

At-A. Comparable, transparent, and reproducible analysis.

Im-H. Lack of acceptance and awareness of biofuels as a viable alternative.

## Project Goal

*Co-Optima Goal:* Advance the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental and economic goals.

*Analysis-Specific Goal:* Guide Co-Optima research and development-guiding through analysis, illuminating scalability and sustainability of co-optimized technologies adopted at scale.

## End of Project Milestone

Analysis has enabled identification of fuel-engine technologies in vehicles with boosted spark-ignition, multi-mode, and mixing controlled compression ignition engines that will lower cost and offers environmental and socio-economic benefits to road transportation.

## Funding Mechanism

Co-Optima Consortium – FY2018 Lab Call

# Additional Slides

# Responses to Previous Reviewers' Comments



<i>Comment</i>	<i>Response</i>
	<p>Generally, the 2019 reviewer comments were positive and as such, the ASSERT Team has followed the course set in the first year of Phase II. TEA and LCA activities have moved forward to address MM and MCCI bioblendstocks. The integrated benefits analysis has incorporated new aspects and expanded models to address diesel heavy duty vehicles per BETO guidance. Refinery analysis has advanced significantly to create new refinery models in PIMS and an accompanying LCA tool and produced results for BSI and MCCI bioblendstocks.</p>
<p>Most existing advanced biofuel processes generate multiple products that are often directed to different markets. There may be value in assessing coproducts as part of this analysis.</p>	<p>Co-products are a key aspect of the process models underlying the TEA and LCA studies. Results have been produced considering co-products, and the size of co-product markets is considered in determining scale up potential. The contribution of co-products to MFSP is explicitly tracked for bioblendstock screening to highlight cases where MFSP is dependent on co-product sales.</p>
<p>Given the potential to adapt/tweak some of the non-favored blendstocks that the Co-Optima team have identified if they offer other benefits (e.g., improved sustainability, etc.), it would be helpful to know if there is a strong GHG LCA or other sustainability reason to focus on the slightly lower priority blendstocks.</p>	<p>The team provides screening results for candidates that meet the screening criteria as well as those that do not. Further information is provided in the Top BSI Bioblendstocks and Top MCCI Bioblendstocks reports to identify promising bioblendstocks that did not fully meet the criteria.</p>





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- Benavides PT, Bartling AW, Phillips S, Singh A, Hawkins TR, Wiatrowski MR, Kinchin CM, Tan ECD, Jones S, Biddy M. Identification of key drivers in techno-economic & life-cycle analysis of MM Co-Optima fuels. *Forthcoming*.

# Publications: Forthcoming Articles



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