DOE Bioenergy Technologies Office (BETO) 2021 Project Peer Review

Techno-Economic and Life Cycle Analysis of Co-Optima Fuels

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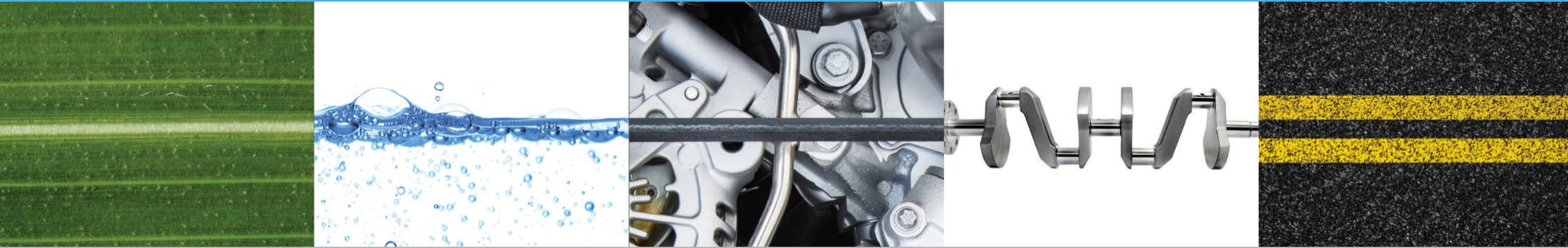
(on behalf of the Analysis Team)

March 15, 2021

CO-OPTIMIZATION OF
FUELS & ENGINES

better fuels | better vehicles | sooner



Project Overview

Task specific goals and expected outcomes

Goals

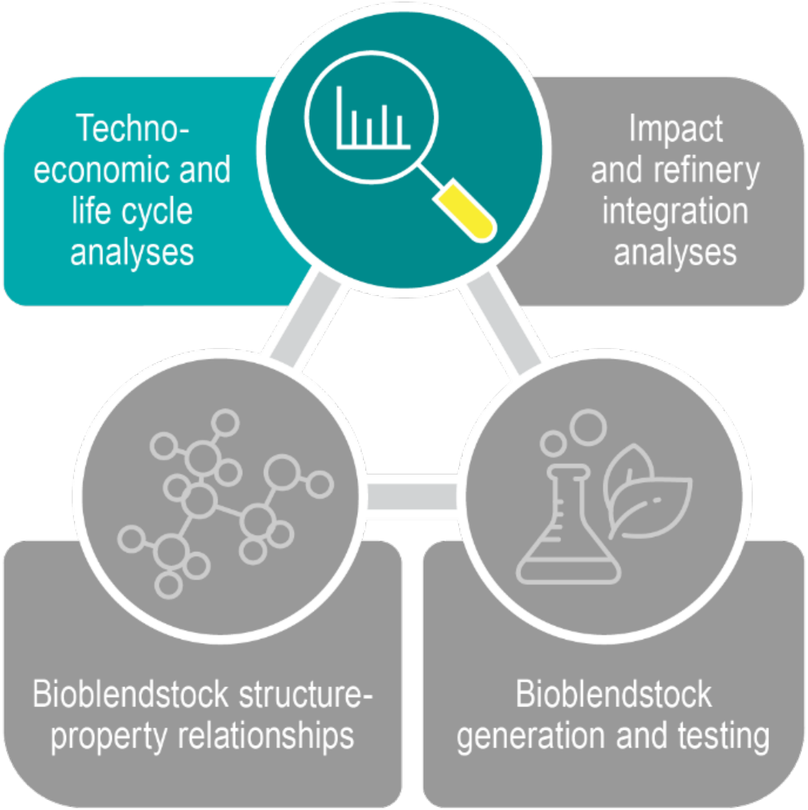
- Evaluate environmental and economic drivers and scalability potential of selected bioblendstocks.
- Identify the most promising fuels for Co-Optima combustion strategies.
  [In collaboration with other teams.]

Impact

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

Relevance

- Addresses BETO goals to increase acceptance of biofuels (Im-H) and provide comparable, transparent, and reproducible analyses (At-A)



Techno-economic and life cycle analyses

Impact and refinery integration analyses

Bioblendstock structure-property relationships

Bioblendstock generation and testing

Project Overview

Guide R&D by identifying low-carbon, cost-effective, and scalable bioblendstocks

- Support Co-Optima's goal to identify fuel-engine combinations that increase fuel economy and reduce emissions.
- TEA and LCA tasks assess the environmental, economic, and scalability considerations for performance-enhancing bioblendstocks.
- Screening-level results are fed back to inform further R&D, rather than assessing at late stage.
- Guides Co-Optima R&D, helps stakeholders understand commercialization potential.
- Significant results are iterated to reduce uncertainty and incorporate additional factors.
- Results disseminated to external stakeholders through publications, presentations, and Co-Optima communications.

Techno-economic and life cycle analyses

Impact and refinery integration analyses

Bioblendstock structure-property relationships

Bioblendstock generation and testing

1. Management

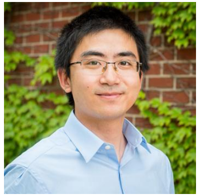
Analysis team members provide necessary breadth and depth of expertise

Troy Hawkins
Team Lead

Avantika Singh
Deputy Team Lead

Andrew Bartling
Task Lead

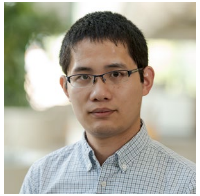
Thathiana Benavides
LCA



Hao Cai
LCA

Experts representing process modeling, TEA, and LCA core capabilities from ANL, NREL, and PNNL

Jennifer Dunn
Advisory
Team Lead Emeritus



Longwen Ou
LCA

Steve Phillips
TEA

Ling Tao
TEA

Greg Zaimes
LCA

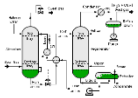
1. Management

Analysis team interfaces with every Co-Optima team as well as the leadership team

Bioblendstock Generation & Testing provides conversion and fuel property data for TEA/LCA and scalability screening

Techno-Economic and Life Cycle Analysis

Process Modeling

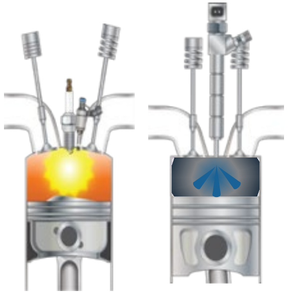


Techno-Economic Analysis

Life Cycle Analysis

Scalability Screening

Analyzing Light and Heavy-Duty Fuels



Light Duty Gasoline Fuels

Heavy Duty Diesel Fuels

Impact and Refinery Integration Analyses environmental and employment effects of scaling up co-optimized fuels and engines, and refiners’ willingness to pay for fuel properties

Structure Property Relationships propose which bioblendstocks are promising to target

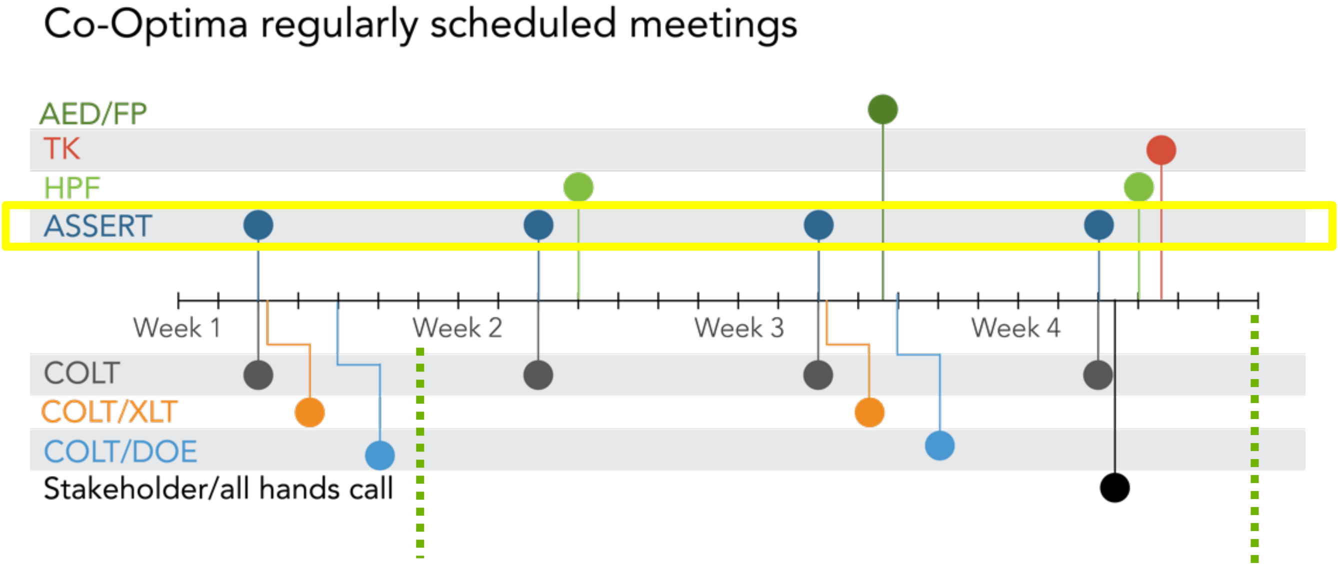
Advanced Engine Development and Toolkit

Provides engine/drivetrain performance

Analysis team estimates economic and sustainability implications

1. Management

TEA and LCA communicate with regularly Co-Optima team and stakeholders



Biweekly Multi-Lab Coordination Calls for TEA-LCA and Waste Pathways Tasks

Analysis Team Monthly Update to DOE and Leadership Team

External Stakeholders

External Advisory Board Quarterly Meetings

Conference Presentations AIChE, ICOSSE, Aachen Fuel Science

Upcoming Co-Optima Capstone Webinars (May, June)

Series of Meetings with Individual Stakeholders

1. Management

TEA and LCA leverages and interacts with other efforts

Co-Optima
TEA and LCA

Leveraging and furthering BETO research

- BETO Multi-Year Program Plans
- Argonne's GREET LCA Model
- Process modeling and TEA at NREL and PNNL
- Expertise from Conversion Program
- Aviation biofuel development
- Feedstock supply research
- Billion Ton Study
- Co-Optima Partner Projects

Interacting with external stakeholders

- External Advisory Board
- California Air Resources Board
- USEPA
- USDA
- Biofuel industry groups
- Petroleum refiners
- OEMs
- Co-Optima publications database
- Conference presentations

1. Management

Planning and milestones guide timely, high quality, impactful outputs

Co-Optima Objectives

Annual Task Plans
and subtask plans

Internal Milestones
ensure timely handoffs

Quality Assurance

External Milestones
key outputs, deliver to DOE

Impact
publications, presentations, stakeholder engagement

- Annual plans focus on Co-Optima objectives
- Data handoff risks managed closely with milestones
- Multi-layered quality assurance
- Planning and coordination lead to impactful deliverables

1. Management

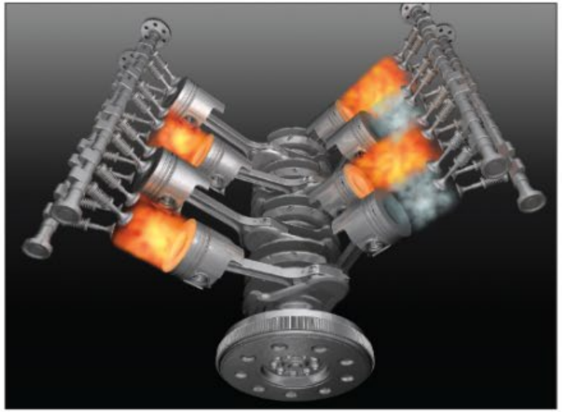
TEA and LCA mitigate risks when developing new bioblendstocks

TEA & LCA Major Risk Factors	**Risk Mitigation Strategy**
Data/information gaps affect the credibility of TEA, LCA, and scalability results	**TEA & LCA** leverage contributing labs' existing models and expertise. Coordinate closely with HPF on production routes and FP to coordinate testing.
Delays in data handoffs from FP and HPF to process modeling/ TEA and from TEA to LCA affect schedule and deliverable quality	**TEA & LCA** communicate regularly with FP and HPF, modeling bioblendstock pathways in batches and triaging high priority pathways

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

TEA & LCA provides metrics for Go/No-Go decisions and benchmarks pathway R&D

Success Metrics for Barrier

Bioblendstock target prices <$5.50/gge

Bioblendstock target GHG reduction >60% relative to conventional gasoline

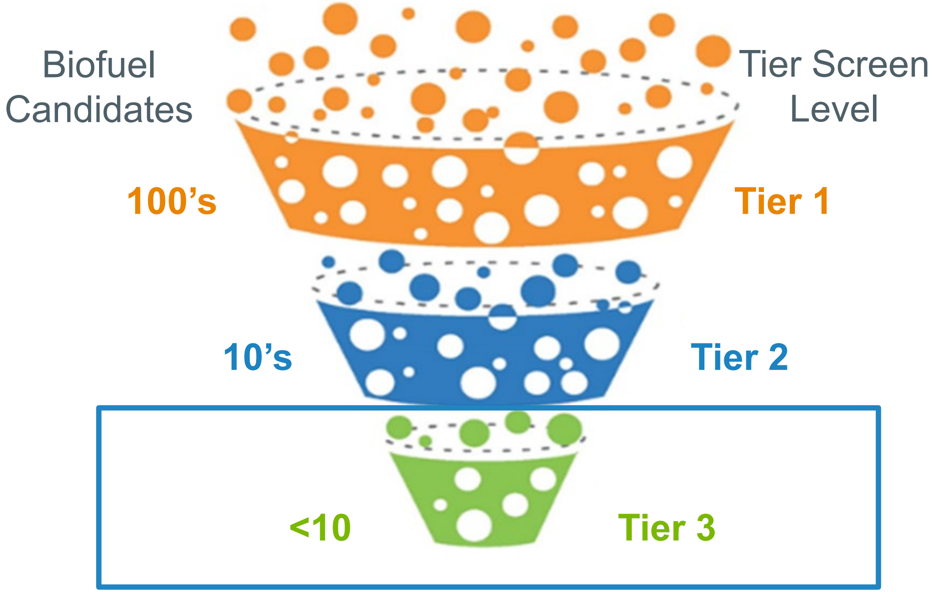
Go/No-Go Decision Points

Bioblendstock pathways that do not meet MFSP and GHG criteria are not pursued further

2. Approach

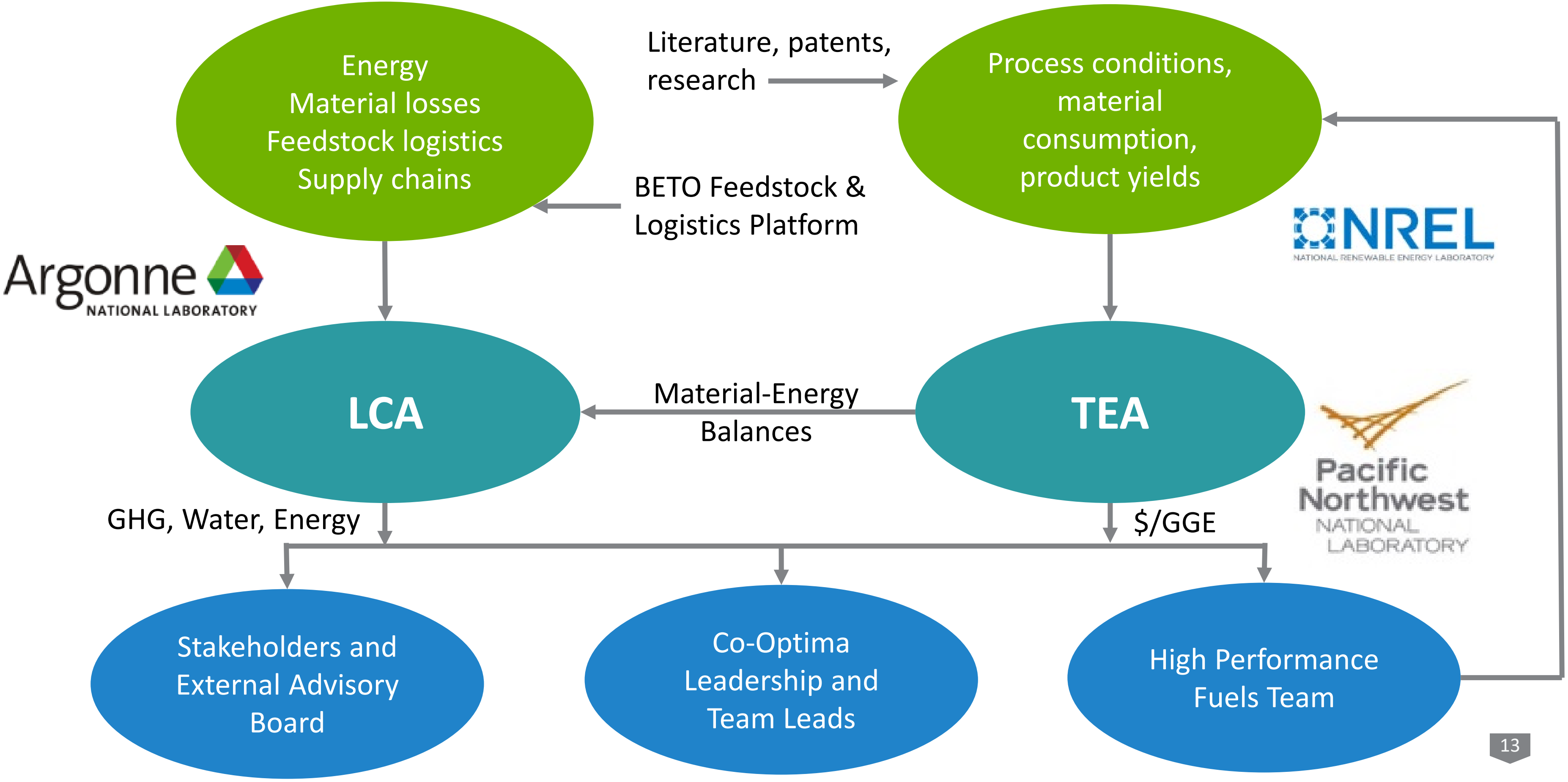
TEA and LCA help identify promising fuels

- Down-select performance enhancing fuels
  - Based on properties from Adv. Engine Dev. 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



2. Approach

Integrated, harmonized TEA and LCA inform Co-Optima research directions



Energy
Material losses
Feedstock logistics
Supply chains

Literature, patents, research

Process conditions, material consumption, product yields

BETO Feedstock & Logistics Platform

LCA

Material-Energy Balances

TEA

GHG, Water, Energy

$/GGE

Stakeholders and External Advisory Board

Co-Optima Leadership and Team Leads

High Performance Fuels Team

2. Approach

TEA and LCA task classify bioblendstocks’ scale up potential

- Economic, environmental, and scalability metrics.
- Current baseline and future target cases
- 19 metrics characterized as
  - Favorable
  - Neutral
  - Unfavorable
  - Unknown

ECONOMICS

ENVIRONMENTAL

Technology Readiness

2. Approach

Bioblendstocks classified based on objective and clearly communicated criteria

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
C efficiency, baseline
C 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

3. Impact As society considers strategies for sustainable transportation, Co-Optima provides insight into the cost-effectiveness of biofuels and optimized engines

Pressure to reduce emissions

- Decarbonization
- Air quality improvements require reducing particulate matter and NO_x

Bio- and waste-based fuels can offer significant GHG reductions

- Co-Optima identifies fuels achieving >60% GHG reductions from gasoline/diesel

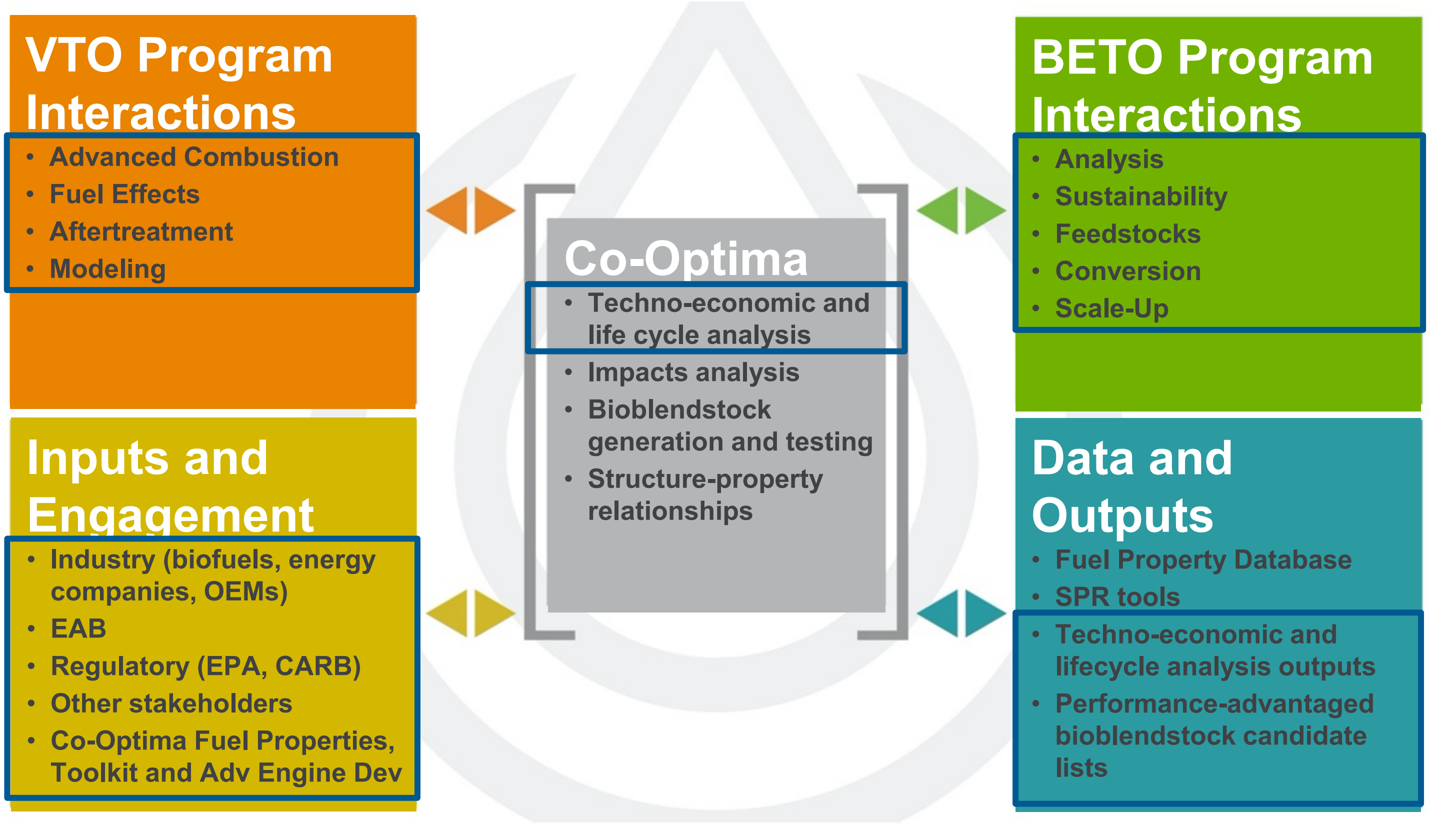
Co-optimized fuels and engines increase efficiency and/or reduce emissions

- Increasing efficiency contributes to climate and air quality objectives for LDVs
- Decreasing engine out PM and NO_x emissions to meet strict future limits for MD/HDVs

Together TEA and LCA provide a cost-benefit perspective

3. Impact

TEA and LCA connects with stakeholders, and the broader BETO and VTO programs



VTO Program Interactions

- Advanced Combustion
- Fuel Effects
- Aftertreatment
- Modeling

Inputs and Engagement

- Industry (biofuels, energy companies, OEMs)
- EAB
- Regulatory (EPA, CARB)
- Other stakeholders
- Co-Optima Fuel Properties, Toolkit and Adv Engine Dev

Co-Optima

- Techno-economic and life cycle analysis
- Impacts analysis
- Bioblendstock generation and testing
- Structure-property relationships

BETO Program Interactions

- Analysis
- Sustainability
- Feedstocks
- Conversion
- Scale-Up

Data and Outputs

- Fuel Property Database
- SPR tools
- Techno-economic and lifecycle analysis outputs
- Performance-advantaged bioblendstock candidate lists

3. Impact

BBG&T impacts community with technical handoffs, engagement, and deliverables

Technical Handoffs

- ✓ Provided economic viability, environmental sustainability, and scalability metrics for **MM and MCCI capstone reports**.
- ✓ Identified Top 10 BSI and Top 12 MCCI pathways for further development through **BETO's Conversion Program**. Top MM pathways forthcoming.
- ✓ Provided TEA and LCA results for **benefits and refinery integration analysis** (next presentation).

Stakeholder Engagement

- ✓ Shared results and received feedback through Co-Optima quarterly External Advisory Board meetings and bi-monthly Stakeholder Calls
- ✓ Strong interest in results from petroleum refiners, OEMs, and biofuel industry
- ✓ Scheduled Co-Optima Capstone webinars to engage with community

Public Facing Deliverables

- ✓ Published 3 papers, with 3 more in preparation, and delivered 5 presentations recently on **TEA and LCA** results
- ✓ Contributed significantly to Co-Optima Year in Review and "Top 10 Boosted SI Bioblendstock" reports that collated major findings across tasks and teams
- ✓ LCA datasets made publicly available in annual GREET update to 40,000+ users

4. Progress and Outcomes

Identified 11 promising MCCI bioblendstocks based on detailed screening of pathways

Environmental results are mixed

- Eleven pathways achieve >60% GHG emission reduction* in target cases
- Only two pathways show favorable LC water usage

Economic metrics largely favorable

- 6 pathways show the potential for target MFSPs of <$4/GGE

New pathways, generally low TRL

- R&D efforts are mostly at bench scale
- More information needed on blend behavior and regulatory limits

*compared with U.S. average conventional diesel

🟢 = 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]	🟢	🔵	🟠	⚪
Long Chain Primary Alcohols	🔵	🟢	🔵	⚪	⚪	⚪	🟠	🟠	🟠	🟢	🟢	🟢	🟠	🟠	0.3	27	🟠	🟠	🔵	4	3	7	3
Long Chain Mixed Alcohols	🔵	🟢	🟢	⚪	⚪	⚪	🟢	🔵	🟢	🟢	🟢	🟢	🔵	🟠	42	42	🔵	🟢	🔵	8	5	1	3
Renewable Diesel via HTL of Wet Wastes	🔵	🟢	🟢	🔵	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	95	107	🟢	🟢	🟢	14	2	0	1
Alkoxyalkanoate Ether-Esters	🔵	🟢	🔵	⚪	⚪	⚪	🟢	🟢	🟢	🟢	🟢	🟢	🔵	🔵	51	71	🟢	🟢	🔵	9	5	0	3
One-Step POMEs from Methanol	🟠	🟢	🟢	🔵	⚪	⚪	⚪	🔵	⚪	🟢	🟢	🟢	⚪	🔵	⚪	52	🟢	🟢	🔵	7	4	1	6
4-Butoxyheptane	🔵	🔵	🔵	🔵	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	40	47	🟠	🔵	🔵	4	8	3	2
Mixed Dioxolanes	🔵	🔵	🔵	⚪	⚪	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟠	43	43	🟠	🟠	🔵	4	6	4	3
Fatty Alkyl Ethers[1]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	232	290	🟢	🟢	🔵	8	4	2	2
Fatty Alkyl Ethers[2]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🟢	🟢	🟢	🟠	🟠	🟢	🟢	210	263	🟢	🟢	🟢	10	3	2	2
Fatty Alkyl Ethers[3]	🔵	🟢	🟢	🔵	⚪	⚪	🔵	🔵	🟢	🟢	🟠	🟠	🟢	🟢	246	308	🟢	🟢	🟠	8	4	3	2
5-Ethyl-4-Propyl-Nonane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟠	35	45	🟠	🔵	🔵	4	8	3	2
4-(Hexyloxyl)Heptane	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🔵	🟢	🟢	🟢	🟢	🔵	🟠	43	47	🟠	🔵	🔵	4	7	4	2
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
Renewable Diesel (HEFA)*	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟢	🟠	🟠	🟢	🟢	224	224	🟢	🟢	🟠	14	0	3	0
Farnesane*	🔵	🔵	🔵	🟢	🟢	🔵	🟠	🔵	🔵	🔵	🟢	🟢	🔵	🟠	30	43	🟢	🟢	🔵	6	9	2	0
Biodiesel (FAME)*	🟢	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🟠	🟠	🟢	🟢	>200		🟢	🟢	🟠	13	1	3	0

1: Feedstock is 60:40 mix of soybean oil and yellow grease
2: Feedstock is 100% yellow grease
3: Feedstock is 100% soybean oil
4: Future target case
5: GGE/dry US ton

MCCI bioblendstock screening results for technology readiness, economic viability, and environmental impact metrics. Routes produced biochemically do not include the valorization of lignin to coproducts. GGE = gasoline gallon equivalent, HTL = hydrothermal liquefaction, LC = life cycle, POME = polyoxymethylene dimethyl ether, HEFA = hydrogenated esters and fatty acids. FAME = fatty acid methyl esters. *Production cost, carbon efficiency, and yield data for these pathways were estimated based on market research and/or prior TEA and may have economic and process assumptions that differ from other bioblendstock pathways evaluated in this figure

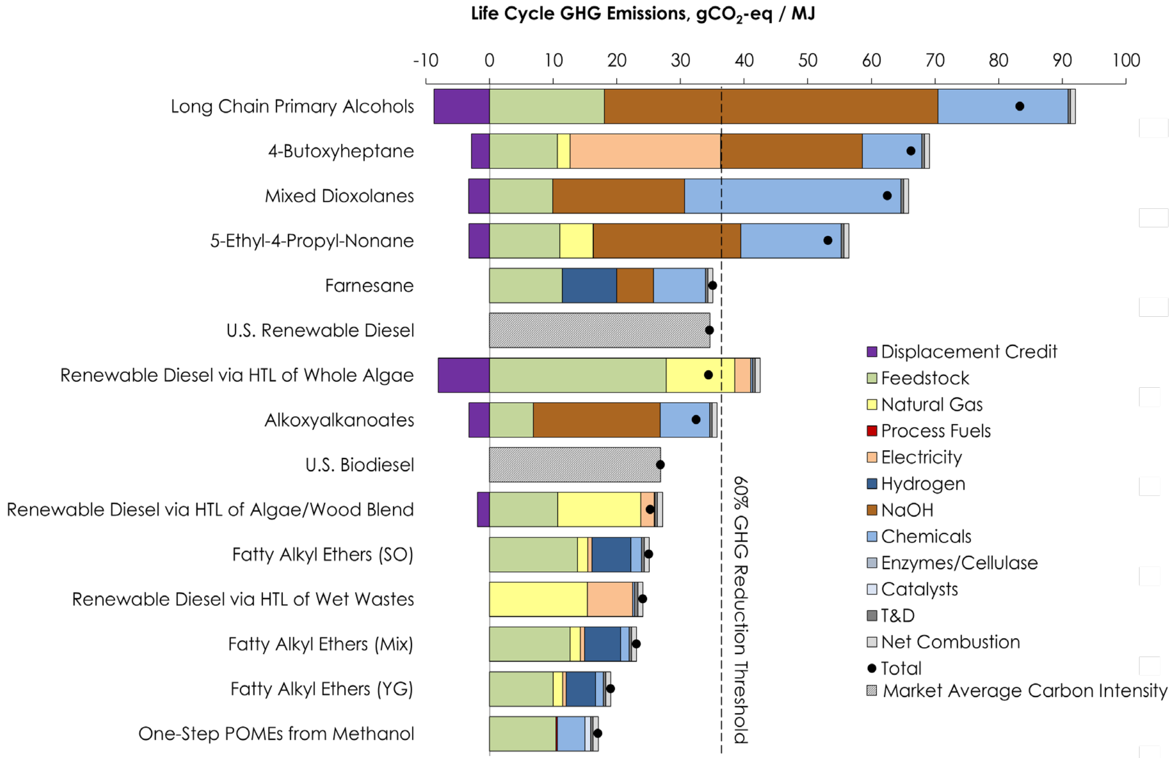
4. Progress and Outcomes Identified 9 MCCI bioblendstocks offering life cycle GHG reductions >60% and highlighted opportunities for improvement

Variety of feedstocks and pathways could provide low C MCCI fuels

Opportunities to improve GHG emissions

- Feedstock production
- NaOH for feedstock pretreatment
- Chemical inputs

*compared with U.S. avg. conventional diesel



Life cycle GHG emissions for MCCI blendstock candidates by GHG source. Purple bars reflect credits associated with displacing emissions for co-products of bioblendstock production. Two blendstocks already on the market (U.S. Renewable Diesel and U.S. Biodiesel) were compared to nine additional candidates SO = soybean oil, YG = yellow grease, Mix = 60:40 mix of SO and YG. The life cycle GHG emissions were evaluated using Argonne National Laboratory's 2020 GREET model.

4. Progress and Outcomes

Bringing down cost is a key challenge for emissions-reducing MCCI bioblendstocks

Feedstock costs contribute significantly to MFSP

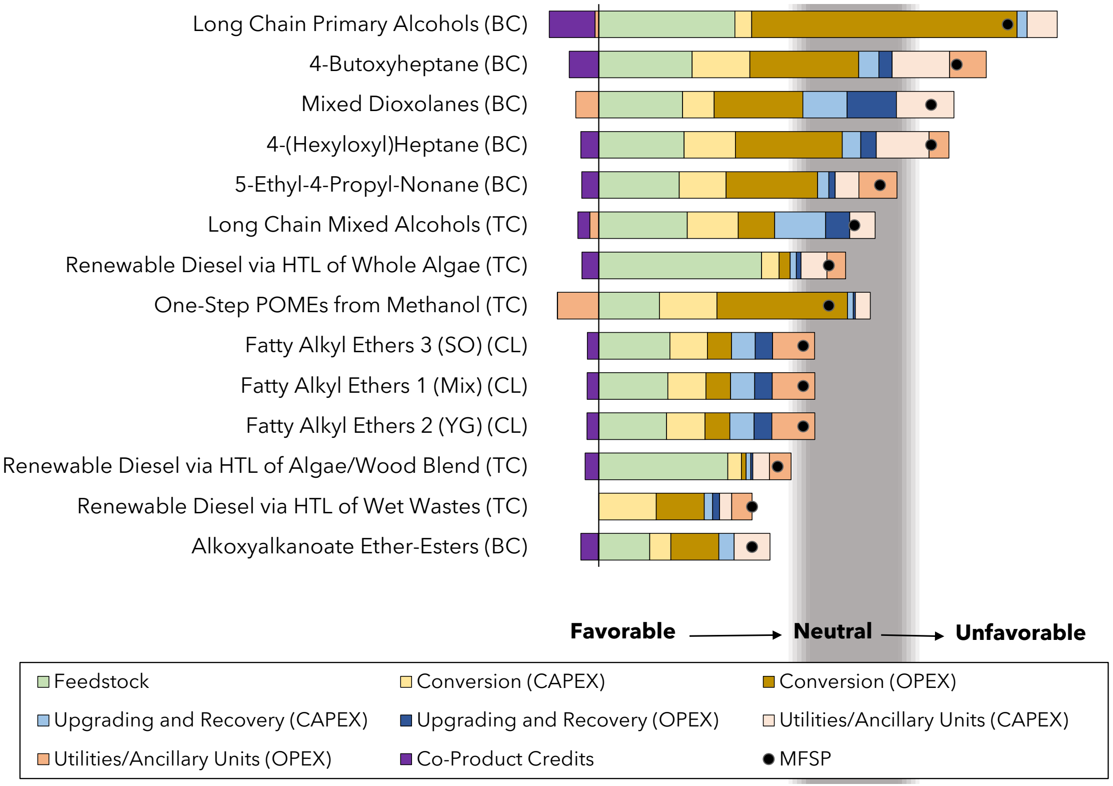
- Identifying waste pathways could reduce cost

Conversion costs highest for biochemical pathways

- Caustic used in pretreatment
- Glucose used in enzyme production

Co-product credits are low

Upgrading and recovery costs typically low



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

4. Progress and Outcomes

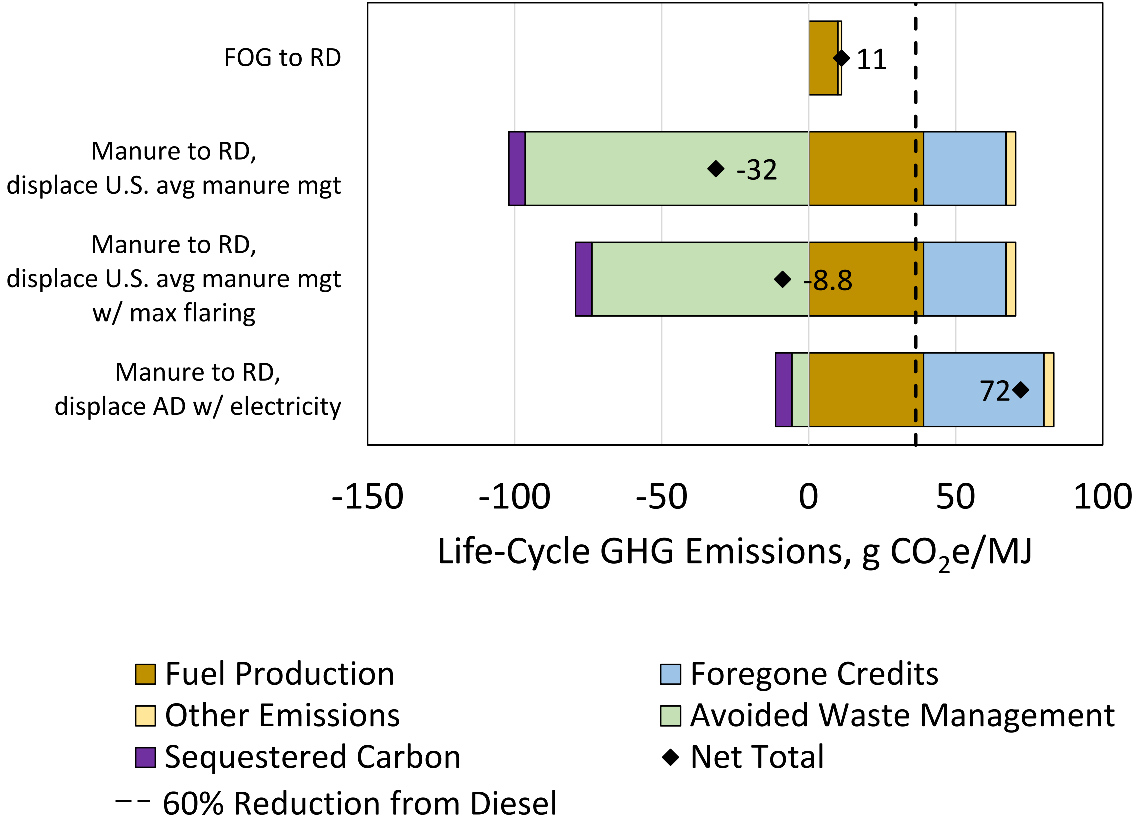
Renewable diesel pathways from waste feedstocks offering very low GHGs for <$5 /gge

Hydrothermal liquefaction of swine manure

- GHG reduction >100%
  due to avoided emissions from manure mgt
- MFSP <$5/gge
- MFSP ~$3.10/gge
  when scaled to 250 tpd

Hydroprocessing of fats, oils, & greases

- GHG reduction ~87%
- MFSP <$5/gge
  potentially lower at larger scale



4. Progress and Outcomes

Identified 10 promising MM bioblendstocks based on detailed screening of pathways

Environmental results consistent

- Pathways selected for >60% GHG emission reduction* in target cases
- Life cycle water use is a potential challenge across all pathways

Economic metrics largely favorable

- Most candidates offer potential MFSPs of <$4/GGE and <$2.50/GGE for methanol.

Technological Readiness Mixed

- Feedstocks available at reasonable costs and in quantities required for scale up.
- Many are already approved fuel additives, although regulations limit blend levels for those with alcohol functional groups.

*Relative to conventional gasoline.

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

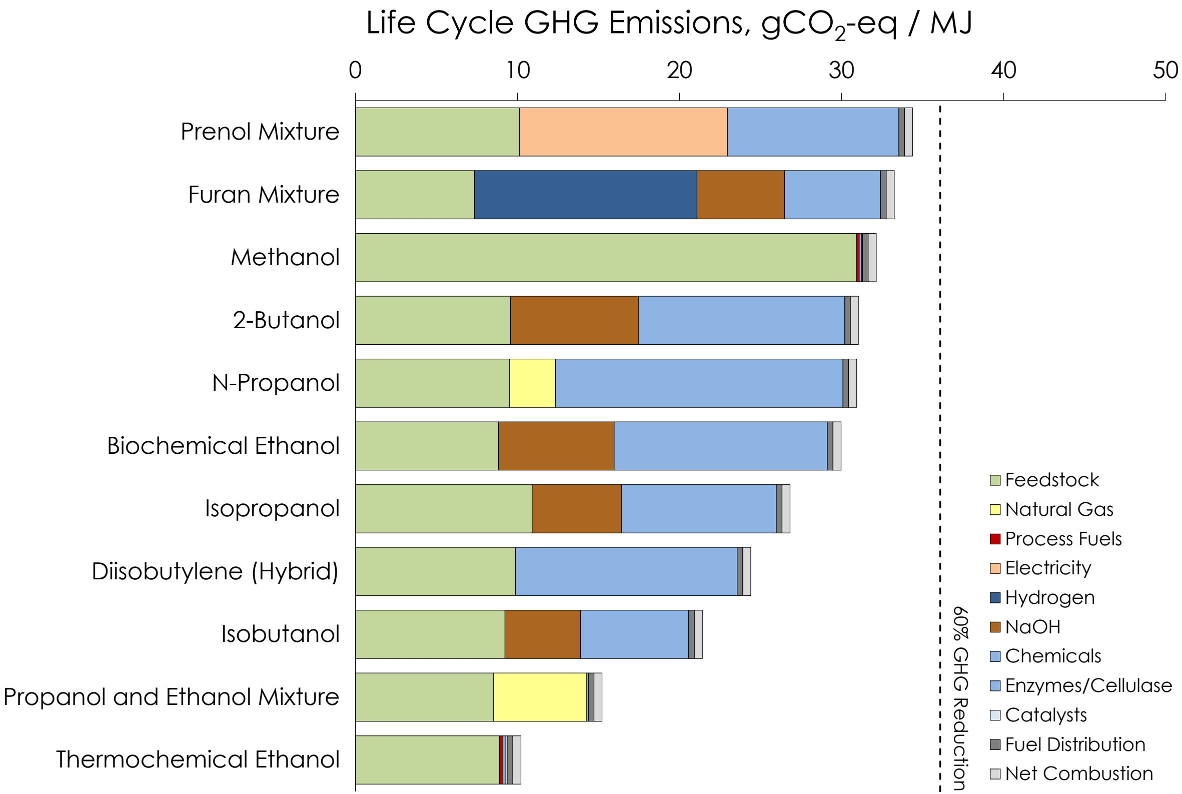
	Technology Readiness						Economic Viability						Environmental							Totals			
	Modeling data source	Fdstk type sensitivity	Fdstk spec sensitivity	Blending behavior	Testing to certification	Blend limit	Blendstock baseline cost	Blendstock target cost	Baseline:target cost	Co-prod dependency	Market competition	Fdstk cost[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	🟢	🟢	🔵	5	9	3	0
2-Methylpropane-1-ol (Isobutanol) (BC)	🔵	🔵	🔵	🔵	🟢	🟠	🔵	🟢	🟢	🟢	🔵	🟢	🔵	🟠	38	49	🟢	🟢	🔵	7	8	2	0
Furan Mixture (2,5-dimethylfuran 2-methylfuran) (BC)	🔵	🔵	🔵	🔵	⚪	⚪	🟠	🟢	🔵	🟢	🔵	🟢	🔵	🟢	31	75	🟢	🟢	🔵	6	8	1	2
Ethanol Reference Case (BC)	🟢	🔵	🔵	🟢	🟢	🔵	🟢	🟢	🟢	🟢	🔵	🟢	🔵	🟠	47	47	🟢	🟢	🔵	10	6	1	0
N-Propanol (BC)	🔵	🔵	🔵	🔵	🟠	🟠	🔵	🔵	🟢	🟢	🔵	🟢	🔵	🟠	33	47	🟢	🟢	🔵	5	9	3	0
Prenol/Isoprenol Mixture (BC)	🔵	🔵	🔵	🔵	⚪	🟠	🟠	🔵	🟠	🟢	🔵	🟢	🟠	🔵	9	49	🟢	🟢	🔵	4	8	4	1
Propanol/Ethanol Mixture (TC)	🔵	🟢	🟢	⚪	🔵	🟠	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🔵	66	67	🟢	🟢	🟢	11	4	1	1
2-Butanol (BC)	🔵	🔵	🔵	🔵	🟠	🟠	🟠	🔵	🟠	🟢	🔵	🟢	🟠	🔵	1	53	🟢	🟢	🔵	4	8	5	0
Methanol (TC)	🟢	🟢	🟢	🔵	🟢	🟠	🟢	🟢	🟢	🟢	🔵	🟢	🟢	🔵	65	65	🟢	🟢	🔵	12	4	1	0
Diisobutylene (Hybrid)	🔵	🔵	🔵	🔵	⚪	🟠	🟢	🟢	🔵	🟢	🟢	🟢	🔵	🟠	39	50	🟢	🟢	🔵	7	7	2	1

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

MCCI bioblendstock screening results for technology readiness, economic viability, and environmental impact metrics. Routes produced biochemically do not include the valorization of lignin to coproducts. GGE = gasoline gallon equivalent, LC = life cycle

4. Progress and Outcomes Identified 9 MM bioblendstocks offering life cycle GHG reductions >60% and highlighted opportunities for improvement

- 10 blendstocks with GHG reductions >60%
  - up to 89%
- Illustrates opportunities for improvement and provides insights into benefits and barriers.
  - Feedstocks
  - NaOH for pretreating feedstock
  - Chemical inputs

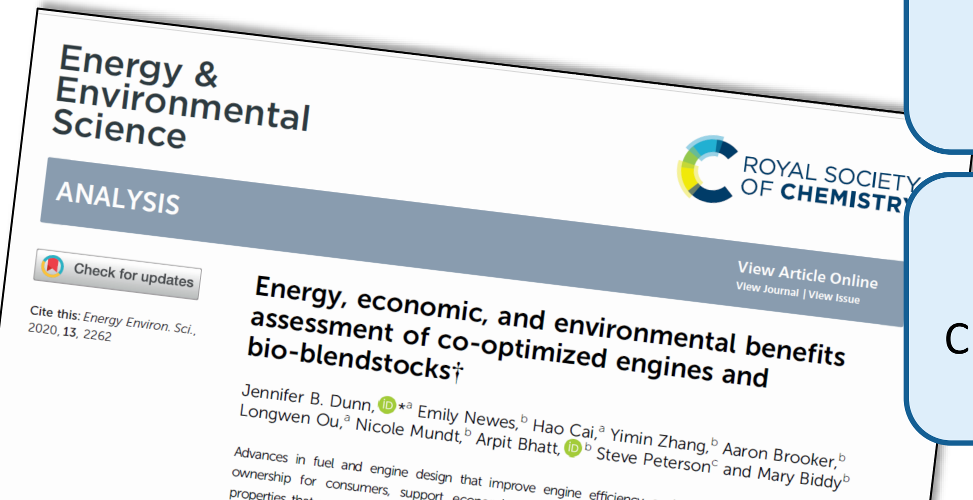


Results are benchmarked against a 60% GHG reduction target relative to baseline petroleum fuel (vertical dashed line). The life cycle GHG emissions were evaluated using Argonne National Laboratory’s 2020 GREET (Greenhouse gases, Regulated Emissions, and Energy use in Technologies) model.

4. Progress and Outcomes

Benefits analysis for BSI, MM, and MCCI

…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†

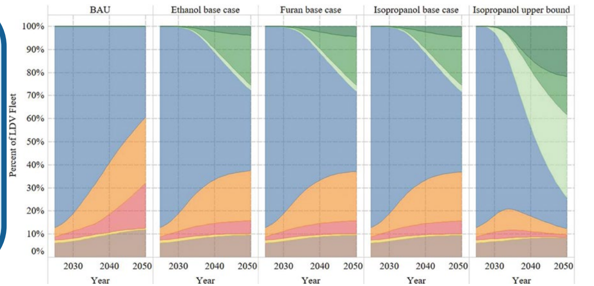
Jennifer B. Dunn, *[a] Emily Newes,[b] Hao Cai,[a] Yimin Zhang,[b] Aaron Brooker,[b] Longwen Ou,[a] Nicole Mundt,[b] Arpit Bhatt, [b] Steve Peterson[c] and Mary Biddy[b]

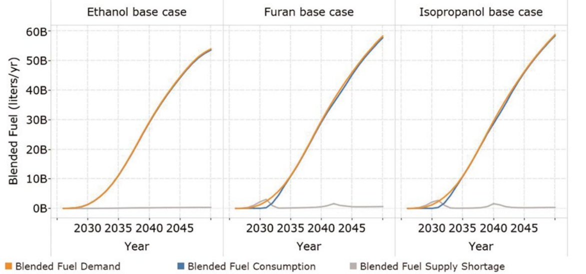
Advances in fuel and engine design that improve engine efficiency
ownership for consumers, support
properties

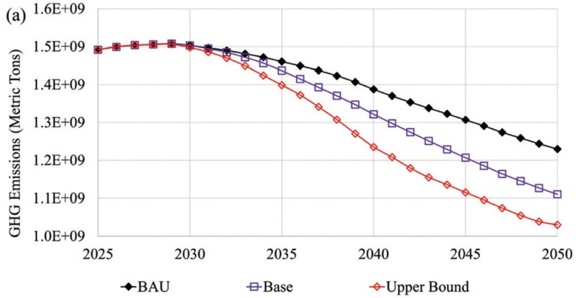
Consumer Choice

Production Capacity

GHG
Water Use
Criteria Pollutants
Jobs







4. Progress and Outcomes

TEA and LCA contributed to achieving Co-Optima goals, provide key feedback to R&D

Light Duty

- 10% fuel economy gain over 2015 baseline

Medium-/Heavy-Duty

- Lower-cost path to reduced engine-out criteria emissions

Biofuels

- Diversify resource base
- Provide economic options to fuel providers to accommodate changing demands and drivers
- Increase market opportunities for biofuels

Crosscutting Goals

- Reduce greenhouse gas emissions by at least 20% for 30% blend of renewable component
- Increase clean energy options and decrease petroleum imports

- Identified cost effective pathways to produce low-carbon, performance advantaged biofuels from terrestrial, waste, and algal biomass.
- Provided comparable, transparent, and reproducible TEA and LCA for bioblendstock production pathways.
- Designed production pathways with potential for 70-90% GHG reductions.*

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*Compared with conventional gasoline or diesel.

5. Summary

Overview	• Analysis supports Co-Optima goals by assessing bioblendstocks across economic, environmental, and scalability metrics. • Screening-level TEA and LCA results are fed back to inform Co-Optima R&D and subsequently refined with additional detail.
Management	• Tasks are well-organized, tracked by milestones, undergo multi-level quality checks. • Interacting with Co-Optima and BETO Teams on common goals and to coordinate efforts. • Regular meetings with External Advisory Board and stakeholders. Disseminating results through articles, reports, and conference presentations.
Approach	• Guide research directions with screening TEA and LCA, iteratively refine results. • Classify bioblendstocks across technological readiness, environmental performance, and economic scalability metrics.
Impact	• Enhance the value proposition for biofuels by identifying scalable, economically viable bioblendstocks that maximize engine performance and energy efficiency and minimize environmental impacts. • Industry regularly expresses strong interest in TEA and LCA to guide biofuel strategies.
Progress & Outcomes	• Completed TEA, LCA, and scalability screening of 13 pathways to produce 9 bioblendstocks for medium-/heavy-duty MCCI engines and 12 pathways to produce 10 bioblendstocks for light-duty MM engines. • Analysis of additional pathways continues in FY21, three journal articles in preparation.

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
DOE Funding	$250K – ANL $255K – NREL $230K – PNNL	$600K – ANL $595K – NREL $570K – PNNL

Partner Labs

- ANL, NREL, PNNL (in coordination with INL, LANL, LBNL, LLNL, NREL, ORNL, PNNL, 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 cost-effective, scalable, and sustainable routes to co-optimized biomass-derived fuels and engines.

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 environmental effects of on road transportation.

Funding Mechanism

Co-Optima Consortium – FY2018 Lab Call

Responses to Previous Reviewers' Comments

Comment	*Response*
	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.
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.	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.
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.	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.

Publications

Journal Articles

J.B. Dunn, E. Newes, H. Cai, Y. Zhang, A. Brooker, L. Ou, N. Mundt, A. Bhatt, S. Peterson, M. Biddy. 'Energy, Economic, and Environmental Benefits Assessment of Co-Optimized Engines and Bio-Blendstocks.' *Energy and Environmental Science*. 2020. 13. 2262-2274.

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Reports

Gaspar D, West BH, Ruddy D, Wilke TJ, Polikarpov E, Alleman TL, George A, Monroe E, Davis R, Vardon D, Sutton AD, Moore CM, Benavides PT, Dunn J, Biddy MJ, Jones SB, Kass MD, Pihl JA, Debusk MM, Sjoberg M, Szybist J, Sluder CS, Fioroni G, Pitz WJ. ‘Top Ten Blendstocks Derived From Biomass For Turbocharged Spark Ignition Engines: Bio-blendstocks With Potential for Highest Engine Efficiency.’ U.S. Dept. of Energy, Office of Energy Efficiency and Renewable Energy. Pacific Northwest National Laboratory. Richland, Washington. PNNL-28713.

Gaspar D, et. al. ‘Top 11 Blendstocks Derived from Biomass for Mixing-Controlled Compression-Ignition (Diesel) Engines: Bioblendstocks with Potential for Decreased Emissions and Increased Operability.’ U.S. Dept. of Energy, Office of Energy Efficiency and Renewable Energy. Pacific Northwest National Laboratory. Richland, Washington. PNNL-XXXXX. (forthcoming)

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Forthcoming Articles

Jiang Y, Phillips SD, Singh A, Jones SB, Gaspar DJ. ‘Economic Values of Low-Vapor-Pressure Gasoline-Range Bio-Blendstocks: Property Estimation and Blending Optimization.’ *In review.*

Cai H, Li S, Tao L, Phillips S, Singh A, Ou L, Hawkins TR. ‘Environmental, Economic, and Scalability of Waste Feedstock-Derived Blendstocks for Mixing-Controlled Compression Ignition Engines.’ *Forthcoming, for submission to Environmental Science and Technology.*

Singh A, Carlson N , Talmadge M, Jiang Y, Sittler L, Brooker A, Zaimes G, Hawkins TR, Newes E., Gaspar D, McCormick, R, Fioni G, Alleman T . ‘Economic Analysis of the Potential Value to Petroleum Refiners for Co-Optima Boosted-SI Bio-Blendstocks.’ *Forthcoming, for submission to Environmental Science & Technology.*

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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

Young B, Hottle T, Hawkins TR, Zaimes G, Chiquelin C, Carlson N, Jiang Y, Talmadge M, Singh A, Dunn J. ‘Environmental Analysis of the Potential Value to Petroleum Refiners for Co-Optima Boosted-SI Bio-Blendstocks.’ *Forthcoming, for submission to Environmental Science & Technology.*

Zaimes G, Hawkins TR, Young B, Singh A, Jiang Y, Talmadge M, Dunn J, Gaspar DJ. ‘Environmental Analysis of the Potential Value to Petroleum Refiners for Co-Optima Boosted-SI Bio-Blendstocks.’ *Forthcoming, for submission to Environmental Science & Technology.*

Sittler L, Brooker A, Zaimes G, Cai H, Longman D, Curran S, Dunn J, Hawkins TR. ‘Synergistic Co-Deployment of Hybridized & Co-Optimized Vehicles,’ *Forthcoming, for submission to Environmental Science & Technology.*

Sittler L, Burli, Hansen S, Newes S, Peterson S. ‘Potential for first mover advantage in new fuel markets.’ *Forthcoming.*

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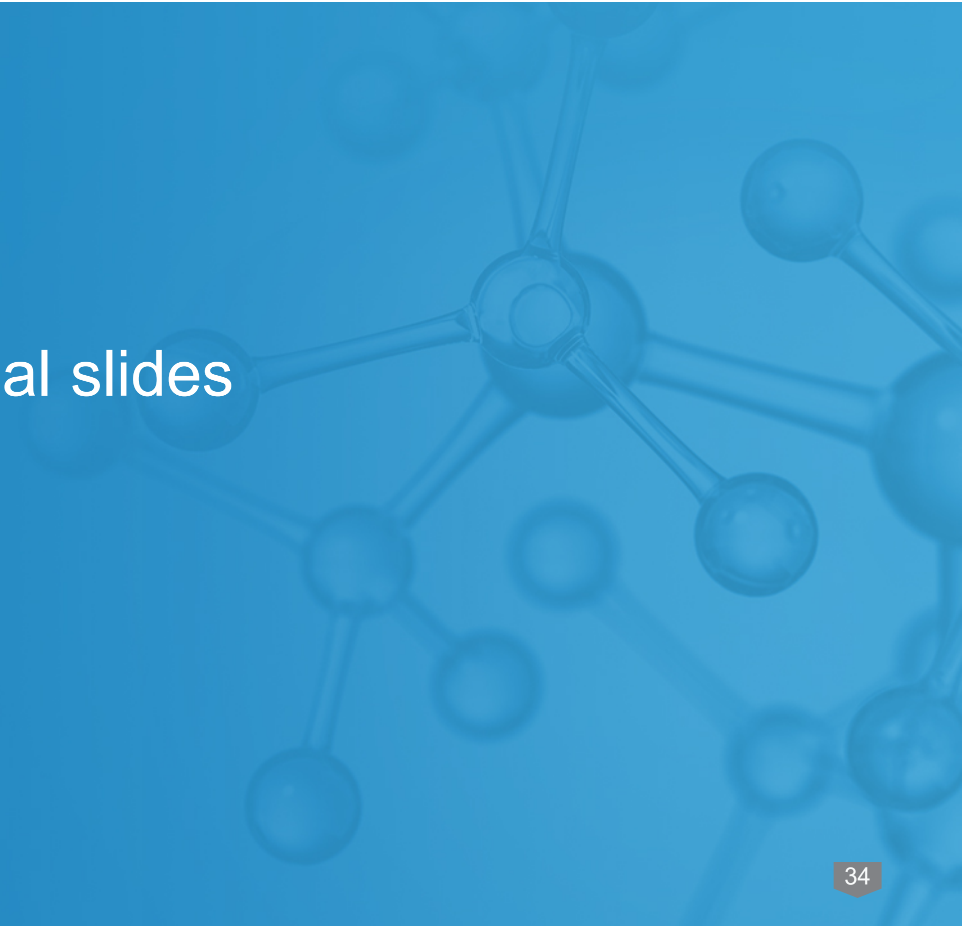
Newes E, Singh A, Sittler L, Talmadge M, ‘Integrating refinery decision logic into bioenergy deployment.’ *Forthcoming.*

Jiang Y, Talmadge M, Singh A, Hawkins TR, Zaimes G, Young B, Ramirez Corredores M, Economic, Energy, and Environmental Analysis of the Potential Value to Petroleum Refiners for Co-Optima MCCI Bio-Blendstocks. *Forthcoming.*



Additional slides

1. Management

Tasks are structured with clear leadership and contributions

	Task Leads, Key Contributors
1. Bioblendstock Techno-Economic Analysis (TEA) and Life Cycle Analysis (LCA) • Process modeling for MM and MCCI bioblendstocks • Estimate minimum fuel selling price • Estimate life cycle GHG emissions, water consumption, and energy use	**Bartling**, Benavides, Phillips, Singh
2. TEA and LCA of Bioblendstocks Produced from Waste	**Cai**, Phillips, Tao
3. Co-Optima Benefits Analysis • Cost benefit analysis of co-optimization of heavy-duty vehicles (FY19-20) • Model updates for infrastructure considerations and for class 8 trucks • MCCI benefits for class 8 trucks and MM benefits for light-duty sector	**Cai**, Newes, Brooker, Sittler, Hawkins, Oke, Zaimes, Avelino, Zhang
4. Synergistic Co-Deployment of Hybridized and Co-optimized Vehicles • Integrated modeling of scaling up co-optimized hybrids (ADOPT, BSM, Bioeconomy AGE, JEDI) • Autonomie Modeling of engine efficiency gains	**Longman**, Brooker, Zaimes, Sittler, Vijayagopal, Newes, Curran, Sluder, Hawkins
5. Economic and Sustainability Benefits of Co-Optima Bioblendstocks for Achieving Desired Fuel Properties at Refineries • Analysis of beneficial fuel properties • Refinery optimization and economic analysis • Life cycle assessment	**Carlson**, Singh, Jiang, Talmadge, Hawkins, Zaimes, Ramirez Corredores

1. Management

Interactions with other Co-Optima teams

High Performance Fuels – Close interaction with process modeling to identify promising production routes for bioblendstocks.

Fuel Properties – Provides candidate biofuels based on interactions with AED Team. Fuel property measurements determine infrastructure compatibility, environmental compliance (e.g. summer smog/Reid Vapor Pressure, water solubility), and energy density considerations.

Advanced Engine Development – Provides engine efficiency and emissions data for specific fuels/fuel properties and combustion strategies. Analysis guides potential for consumer adoption of co-optimized drivetrains and cost and environmental comparison to conv. fuels.

Toolkit – Provides estimated engine performance prior to engine testing. Incorporation of economic and sustainability aspects in their modeling.

Co-Optima Leadership – Regular interactions to understand analysis results to guide R&D and to make connections between analysis and new R&D developments.

External Advisory Board – Quarterly and ad hoc meetings guide analysis directions and provide insights for extending analyses.

1. Management

Coordination, collaboration, and communication

Coordination and Collaboration

- **ASSERT Team:** Weekly meeting for whole team coordination, including Co-Optima Leadership Team and DOE Technical Managers.
- **Task Teams:** meet on a biweekly basis. Numerous other interactions occur as needs arise.
- **Co-Optima Coordination:** Team Leads represent ASSERT at Co-Optima Extended Leadership Team, External Advisory Board, and Stakeholder meetings.
- **Other Co-Optima Teams:** Regular check-ins to coordinate, e.g. interactions with Fuel Properties Team around list of candidate bioblendstocks for further down-selection.

Communication

- **Monthly Updates:** Provided to Co-Optima Team and DOE/lab stakeholders, including an extended highlight on a different ASSERT Team activity each month together with updates from each individual task. Reviewed with other teams at monthly Leadership Team Meeting.
- **Presentations:** ASSERT Team members present at relevant conferences. Updates provided on bi-monthly Co-Optima Stakeholder calls. Meetings by request with interested stakeholders happen regularly.
- **Peer-Reviewed articles and Reports**

2. Approach Bioblendstocks classified based on objective and clearly communicated criteria: Technology readiness metrics

Metric	**Favorable (+)**	**Neutral (0)**	**Unfavorable (-)**
Process modeling data source	Demonstration-scale (or larger) data available, this includes detailed process analysis from literature	Bench-scale data available	Notional, yields and conversion conditions estimated partly from literature
Production process sensitivity to feedstock type	Feedstock changes result in *minor variations* in fuel yield/quality	Feedstock changes result in *some variations* in fuel yield/quality	Feedstock changes can cause *significant variations* in fuel yield/quality
Robustness of process to feedstocks of different specs	Changes in feedstock specifications *minimally* influences yield/quality	Changes in feedstock specifications *moderately* influences yield/quality	Changes in feedstock specifications *greatly* influences yield/quality
Blending behavior of bioblendstock with current fuels for use in vehicles	Current quality good enough for replacement (i.e. drop-in)	Current quality good enough for blend	Current quality in blend not good or unknown
Bioblendstock underwent testing towards certification	Yes	Limited	None
Bioblendstock will be blendable only in limited levels because of current legal limits	No limit	Blendable at high levels	Significant limit (i.e. on aromatics)

2. Approach Bioblendstocks classified based on objective and clearly communicated criteria: Economic viability metrics

Metric	Favorable (+)	Neutral (0)	Unfavorable (-)
Co-Optima bioblendstock production baseline cost	Falls in cluster of lowest cost pathways (≤$5/GGE)	Falls in cluster of moderate cost pathways ($5/GGE - $7/GGE)	Falls in cluster of high cost pathways (≥$7/GGE)
Fuel production target cost	Falls in cluster of lowest cost pathways (≤$4/GGE)	Falls in cluster of moderate cost pathways ($4/GGE - $5.5/GGE)	Falls in cluster of high cost pathways (>$5.5/GGE)
Ratio of baseline-to-target cost	<2	2–4	>4
Percentage of product price dependent on co-products (i.e., chemicals, electricity, other bioblendstocks/fuels produced as co-product to Co-Optima fuel)	<30%	30–50%	>50%
Competition for the biomass-derived bioblendstock or its predecessor	Bioblendstock is not produced from, nor is itself, a valuable chemical intermediate	Bioblendstock is produced from, or is itself, a raw chemical intermediate	Bioblendstock is produced from, or is itself, a valuable chemical intermediate
Cost of feedstock (in US$2016)	Cost likely to be at or below target of $84/dry ton delivered at reactor throat	Cost likely to be between $84/dry ton to $120/dry ton delivered at reactor throat	Cost likely to exceed $120/dry ton delivered at reactor throat

2. Approach Bioblendstocks classified based on objective and clearly communicated criteria: Environmental sustainability metrics

Metric	Favorable (+)	Neutral (0)	Unfavorable (-)
Baseline: Efficiency of input carbon (fossil and biomass-derived) to Co-Optima bioblendstock	>30%	10–30%	<10%
Target: Efficiency of input carbon (fossil and biomass -derived) to Co-Optima bioblendstock	>40%	30–40%	<30%
Baseline: Co-Optima bioblendstock yield (GGE/dry ton)*			
Target: Co-Optima bioblendstock yield (GGE/dry ton)*			
Target: Life-cycle GHG emission reduction compared to conventional diesel fuel	≥60%	50% - 60%	<50%
Target: Life-cycle fossil energy consumption reduction compared to conventional diesel fuel	≥60%	50% - 60%	<50%
Target: Life-cycle water consumption	≤3 gal/GGE	3 gal/GGE - 55 gal/GGE	>55 gal/GGE

* Baseline and target bioblendstock yields were included for reference, but were not ranked on favorability due to different comparative bases on pathways and feedstocks

2. Approach

List of bioblendstocks evaluated

Bioblendstock	Pathways	Feedstock
Long Chain Primary Alcohols	[B] Biochemical fermentation to products	Corn Stover
Long Chain Mixed Alcohols	[B] Biochemical fermentation to ethanol with catalytic upgrading	Corn Stover
Renewable Diesel via HTL of Wet Wastes	[T] Thermochemical via hydrothermal liquefaction with hydrotreating	Wet Waste (Sludge)
Hydroxyalkanoate-Based Ethyl-Esters	[B] Biochemical fermentation to alcohols and lactic acid with catalytic upgrading of intermediates	Corn Stover
One-Step OMEs from Methanol	[T] Thermochemical methanol via syngas with further synthesis to OMEs	Forest Residues
4-Butoxyheptane	[B] Biochemical fermentation to carboxylic acids with catalytic upgrading	Corn Stover
Mixed Dioxolanes	[B] Biochemical fermentation to ethanol and BDO with catalytic upgrading	Corn Stover
Fatty Acid Ethers (1)	Catalytic upgrading of biodiesel	60:40 Mix Soy Oil:Yellow Grease
Fatty Acid Ethers (2)	Catalytic upgrading of biodiesel	100% Yellow Grease
Fatty Acid Ethers (3)	Catalytic upgrading of biodiesel	100% Soybean Oil
5-Ethyl-4-Propyl-Nonane	[B] Biochemical fermentation to carboxylic acids with catalytic upgrading	Corn Stover
4-(Hexyloxyl)Heptane	[B] Biochemical fermentation to carboxylic acids with catalytic upgrading	Corn Stover
Upgraded Pyrolysis Oils	[T] Thermochemical to pyrolysis oils with hydrotreating	Clean Pine
Renewable Diesel via HTL of Whole Algae	[T] Thermochemical via hydrothermal liquefaction with hydrotreating	Algae

For this analysis, biochemical pathways assume lignin is burned for process heat and not upgraded to valuable co-products.
[B]: Biochemical pathway, [T]: Thermochemical pathway