Co-Optima Program: Potential Impact at Scale

Avantika Singh
National Renewable Energy Laboratory
(on behalf of the Analysis Team)
March 15, 2021
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
Analysis team interacts with every Co-Optima team and guidance from leadership team

**Advanced Engine Development**
Provides engine efficiency & emissions data for fuels/combustion strategies

**Vehicle Adoption**
Analysis team estimates economic and sustainability implications

**Toolkit Development**
Provides estimated engine performance prior to engine testing

**High Performance Fuels**
Identify bioblendstock pathways & provide conversion data

**Fuel Properties**
Inputs on relevant fuel properties and their blending with conventional fuels

- **Economy-wide Benefits**
  - Considering both LD and HD modes

- **Techno-economic and life cycle analyses**
  - Refinery Impact Analysis
  - Vehicle Adoption
  - Economy-wide Benefits

- **Impact and refinery integration analyses**

Light Duty Gasoline Fuels
Heavy Duty Diesel Fuels
1. Management

Analysis experts representing core capabilities from different national labs

Troy Hawkins (Lead)

Avantika Singh (Deputy Lead)
1. Management
Coordination, Collaboration, and Communication

Co-Optima regularly scheduled meetings

AED/FP
TK
HPF
ASSERT

Week 1
Week 2
Week 3
Week 4

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

Stakeholder/all hands call
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.

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

**Risk Mitigation Strategy**

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

- 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

**Heavy Duty**
- Cetane
- Energy Density
- Flash / Boil / Freeze
- RVP / HOV
- Water Solubility
- Sooting

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

2. Approach: Refinery Impact Analysis
Quantifies potential bio-blendstock value to refiners using linear programming tools

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

Petroleum Crude Oils → 

Petroleum Refinery

- Atmospheric and Vacuum Distillation
- Delayed Coking
- Fluid Catalytic Cracking
- Kerosene/Jet Hydrotreating
- Naphtha Hydrotreating
- Isomerization
- Naphtha Reforming

+ Hydrocracking
+ Diesel Hydrotreating
+ Gasoline Hydrotreating
+ Alkylation

Co-Optima Bio-Blendstocks

BUY

Finished Fuels and Products

→ Regular Gasoline (C/R)
→ Premium Gasoline (C/R)
→ Co-Optima Boosted SI
→ Jet Fuel and Kerosene
→ Ultra-Low Sulfur Diesel
→ Heating and Marine Fuels
→ Other Refinery 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

- Aspen PIMS
  By AspenTech

Life Cycle Analysis
2. Approach: Refinery Impact Analysis

Developed LCA tool coupled with refinery models to measure environmental benefits

Bio-blendstock Cases
- Ex: Soybean Diesel

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
  - VOC emissions from tanks and fugitives

Excel based tool to inform carbon intensity of refinery emissions

PIMS-LCA
- (Case Comparison)

- Refinery Overview
  - (Crude, Product)

- Refinery-Wide Impacts
  - (Product, Source)

- Per Unit Product Impacts
  - (Emissions Species, TRACI Impact, Supply Chain Segment)

- End-use Emissions
  - (Sector, Technology)

Environmental performance comparison across BAU and BBS Scenarios
2. Approach
Integrated modeling tools for measuring potential impact of light and heavy-duty modes

**Light Duty**
- RON / MON / S
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- Sooting

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

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

2. Approach: Vehicle Adoption
Market factors considered in evolution of Co-Optima vehicles in the automobile fleet

1. All Existing Makes/Models

2. Consumer Preferences
   - Nonlinear
   - Price dependent

3. Regulations
   - CAFE
   - GHG Rule
   - Incentives

Benefits offered by Co-Optima technology

Technology Improvements

Validation

Market Driven Future Options
2. Approach
Integrated modeling tools for measuring potential impact of light and heavy-duty modes

Light-Duty and Heavy-Duty Fuels and Combustion Modes

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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: 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?

Value Proposition
Example: Aftertreatment cost benefit analysis

TEA
Fuel selling price of biofuels?

BSM
How will the biofuels industry grow?

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

Bioeconomy AGE
Energy and environmental impacts of biofuels

GREET
Emissions, water, and energy intensity of fuels

BEIOM
What are the economic impacts from biofuel plant construction?

Biofuel selling price of biofuels?

Feedback between co-optimized blended fuel price and impact on sales of next year's co-optimized vehicles

What feedstock growth is required to meet demand?

How many biorefineries need to be constructed to meet demand?

How much co-optimized vs conventional fuel is consumed

How will the vehicle/fuel markets evolve over time?

Volume of fuel consumed by type

Vehicle fleet composition (including co-optimized hybridized vehicles)

Vehicle ownership cost reduction

Reduction in urea use

Life cycle fossil energy use, water consumption, greenhouse gas emissions, and air pollutant emissions intensities of biofuels and conventional fuels

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

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

Gross/net job benefit vs time associated with co-optimized vehicle/fuel deployment

Energy, material flows

Energy and environmental impacts of biofuels

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

Vehicle fleet composition

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

Vehicle fleet composition (including co-optimized hybridized vehicles)

Vehicle fleet composition

Vehicle fleet composition (including co-optimized hybridized vehicles)
3. Impact
Co-Optima connects with stakeholders, and the broader BETO and VTO programs

VTO Program Interactions
- Advanced Combustion
- Fuel Effects
- Aftertreatment
- Modeling

BETO Program Interactions
- Analysis
- Sustainability
- Feedstocks
- Conversion
- Scale-Up

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

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

<table>
<thead>
<tr>
<th>Outcome &amp; Impact</th>
<th>Stakeholder Engagement</th>
<th>Disseminating Results</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Outcome</strong>: Information on scalability, economic viability, and environmental/socio-economic benefits of low carbon bioblendstocks</td>
<td>✓ Attend Co-Optima quarterly <em>External Advisory Board</em> meetings</td>
<td>✓ Journal Articles (3 published, 9 in preparation) and several conference presentations</td>
</tr>
<tr>
<td><strong>Impact</strong>: Estimated potential impact of Co-Optima technology adoption at scale, with demonstrated <em>engine efficiency improvements, emission reductions, &amp; domestic job growth</em></td>
<td>✓ Share results and receive feedback from <em>leadership team</em> and the <em>Board of Directors</em></td>
<td>✓ Annual Co-Optima Year in Review and other reports collating major findings</td>
</tr>
<tr>
<td></td>
<td>✓ Present research findings at the monthly <em>Co-Optima stakeholder</em> calls</td>
<td>✓ Co-Optima Capstone webinars scheduled on LD and HD sector benefits</td>
</tr>
</tbody>
</table>
4. Progress and Outcomes: Light Duty Sector
Integrated modeling tools for measuring potential impact of light- and heavy-duty modes

Light-Duty and Heavy-Duty Fuels and Combustion Modes

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

**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?
4. Progress and Outcomes: Refinery Impacts (LD)
Blending optimization estimated economic value of Co-Optima bioblendstocks

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**

Jiang, Philips, Singh, Gaspar et al. (2021) in revision
Fuel characteristics (RON and S) of Co-Optima biofuels drive economic benefits to refiners.

**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**.

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.

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

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

*Sittler, Zaimes, Brooker, Longman et al. (2021) in preparation*
4. Progress and Outcomes: Heavy Duty Sector
Integrated modeling tools for measuring potential impact of light- and heavy-duty modes

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

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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

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-Opima 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

**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

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**Properties**

- 2-Nonanol
- Methyl decanoate
- Dipentyl ether
- 4-butoxy heptane
- 5-ethyl-4-propyl-nonane
- Soy biodiesel
- HTL diesel
- OMEs

**Break-even Value of MCCI Bio-Blendstocks ($/bbl)**

<table>
<thead>
<tr>
<th>Properties</th>
<th>10 vol% w/ CDF</th>
<th>30 vol% w/ CDF</th>
<th>10 vol% BC</th>
<th>30 vol% BC</th>
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</thead>
<tbody>
<tr>
<td>Diesel Price</td>
<td>150</td>
<td>120</td>
<td>120</td>
<td>120</td>
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<tr>
<td>ULSD Spec</td>
<td>&gt;40</td>
<td>&gt;40</td>
<td>&gt;40</td>
<td>&gt;40</td>
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<tr>
<td>CDF Spec</td>
<td>&gt;53</td>
<td>&gt;53</td>
<td>&gt;53</td>
<td>&gt;53</td>
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</tbody>
</table>

**Cetane number**

<table>
<thead>
<tr>
<th></th>
<th>ULSD Spec</th>
<th>CDF Spec</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Nonanol</td>
<td>38-41</td>
<td>46-52</td>
</tr>
<tr>
<td>Methyl decanoate</td>
<td>91-96</td>
<td>57-65</td>
</tr>
<tr>
<td>Dipentyl ether</td>
<td>48</td>
<td>54-55</td>
</tr>
<tr>
<td>4-butoxy heptane</td>
<td>65.8</td>
<td>93</td>
</tr>
<tr>
<td>5-ethyl-4-propyl-nonane</td>
<td>48</td>
<td>54-55</td>
</tr>
<tr>
<td>Soy biodiesel</td>
<td>65.8</td>
<td>93</td>
</tr>
<tr>
<td>HTL diesel</td>
<td>65.8</td>
<td>93</td>
</tr>
<tr>
<td>OMEs</td>
<td>48</td>
<td>54-55</td>
</tr>
</tbody>
</table>

**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

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*Jiang, Carlson, Singh, et al. (2021) in preparation*
4. Progress and Outcomes: Refinery Impacts (HD)

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

For Diesel blended with soy biodiesel, GHG emissions range from net negative to higher than ULS Diesel over the range of blend levels.

Key Outcome:

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

Co-Optima Project: Accomplishments

Provide technology options to increase sustainability of transportation

**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

**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
## 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

<table>
<thead>
<tr>
<th>FY20</th>
<th>Active Project</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Funding</td>
<td>$1,700K</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Comment</th>
<th>Response</th>
</tr>
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<tbody>
<tr>
<td>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.</td>
<td></td>
</tr>
<tr>
<td>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.</td>
<td>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.</td>
</tr>
<tr>
<td>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.</td>
<td>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.</td>
</tr>
</tbody>
</table>


Publications: Forthcoming Articles


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