Co-Optimization of Fuels & Engines

DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

Integrated analysis of efficiency-enhancing bio-blendstocks

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Co-Optima

Jennifer Dunn
Argonne National Laboratory

Mary Biddy
National Renewable Energy Laboratory

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Goal Statement

Goal:

- *Evaluate co-optimized bio-blendstock and engine technologies from an environmental and economic perspective while conducting research and development-guiding analyses.*

Outcome:

- *Co-Optima teams gain insight into the value proposition of co-optimized fuels and engines and routes to overcome environmental and economic barriers to their realization.*

Relevance:

- *Disseminate information on scalability, economic viability, and environmental sustainability of bio-blendstocks that may be of interest to industry.*
- *Outline key economic and sustainability drivers and barriers for moving fuels to market to guide Co-Optima's overall relevance to industry.*

Quad Chart Overview

Timeline

Project start: FY2016
Merit Review Cycle: FY2019 to FY2021
12% completion of review cycle

	Total Costs Pre FY17	FY 17 Budget	FY 18 Budget	Total Planned Funding (FY 19-Project End Date)
BETO Funding	$3,631	$3,120	$3,394	$9,375

Partners: ANL, NREL, PNNL, SNL
VTO does not fund ASSERT.

Barriers

ADO-E: Co-Development of Fuels and Engines
At-A: Analysis to inform strategic direction

Objective

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 Goal

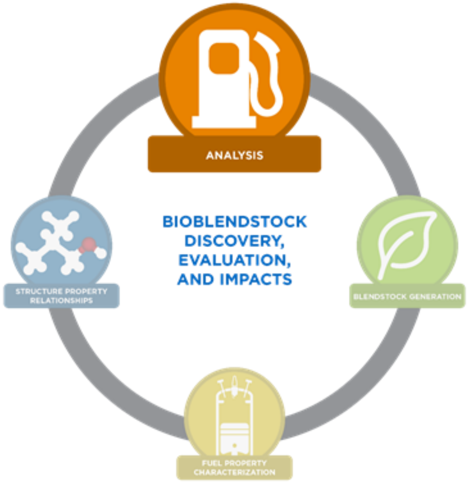
ASSERT analyses have enabled identification of fuel-engine technologies in vehicles with boosted spark-ignition, MCCI, multi-mode and advanced compression ignition engines that will lower cost and environmental effects of on road transportation.

ASSERT: Analysis of Sustainability, Scale, Economics, Risk and Trade

1 - Project Overview

ASSERT Overview

- Co-Optima’s overall goal is to identify low carbon fuel-engine combinations that increase fuel economy by 35% (light duty) or 4% (heavy duty) over a 2015 baseline, with reduced emissions
- The ASSERT* team supports Co-Optima goals by:
  - Evaluating environmental and economic drivers and the scalability potential of perspective bio-blendstocks
  - Sharing these key outputs with the teams and stakeholders
  - Guiding Co-Optima’s research and development
- ASSERT assesses potential benefits or drawbacks of deploying co-optimized fuels and engines in the transportation sector with respect to:
  - Energy consumption
  - Influence on refineries
  - Air pollutant emissions and water consumption
  - Job creation
  - Technology readiness for scale up in the near term
  - Economic viability



*Analysis of Sustainability, Scale, Economics, Risk and Trade

2 – Approach (Management)

Approach (Management)

- The ASSERT team is led by Jennifer Dunn at Argonne National Laboratory and Mary Biddy at the National Renewable Energy Laboratory
- Team members have expertise in the **crosscutting** areas of
  - Techno-economic analysis (TEA) (NREL, PNNL)
  - Life cycle analysis (LCA) (ANL)
  - Refinery modeling (ANL, NREL, PNNL)
  - Job creation modeling (NREL)
  - Modeling of expansion of biofuels industry in response to demand (NREL)
  - Vehicle fleet sector evolution upon introduction of new vehicle technologies (ANL, NREL)
- The team holds weekly conference calls and has participants on the HPF team calls with strategic communications with other teams
- The team leadership convenes monthly with the Leadership Team to gauge analysis needs of the program for project planning and impact as well as to brief leadership on recent progress and receive feedback.

Approach (Management)

Biorefinery

Petroleum Refinery Integration

Fuel Distribution

Fueling Infrastructure

- ASSERT incorporates expertise covering the biofuel supply chain, leveraging feedstock platform analysis and insights
- Examples of integration with other teams

High Performance Fuels: Information exchange regarding route to producing blendstock candidates and their properties. Regular participation on conference calls. Team lead meetings held as needed for specific tasks.

Fuel Properties: Information exchange regarding fuel properties, especially blended fuels

Toolkit Team: Collaboration regarding use of economic and sustainability aspects of blendstock candidates in their modeling

Advanced Engine Development Team: Seek input regarding modeling assumptions such as engine efficiency gains, aftertreatment device performance

Leadership Team: Monthly calls to gain insights into analysis direction and overall Co-Optima analysis needs, provide results updates

Team Members

FY18-19 ASSERT Team Members

- ANL: ***Jennifer Dunn***, Hao Cai, Jeongwoo Han, Doug Longman, Thathiana Benavides, Longwen Ou, Marianne Mintz
- NREL: ***Mary Biddy***, Emily Newes, Aaron Brooker, Teresa Alleman, Kristi Moriarty, Margo Melendez, Yimin Zhang, Avantika Singh, Jennifer Clippinger, Andrew Bartling, Matthew Wiatrowski, Ryan Davis, Abhijit Dutta, Eric Tan, Christopher Kinchin
- PNNL: ***Sue Jones***, George Muntean, Steven Phillips, Yuan Jiang
- SNL: ***Paul Bryan***

Sandia National Laboratories

Pacific Northwest NATIONAL LABORATORY

Argonne NATIONAL LABORATORY

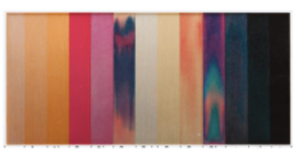
NREL NATIONAL RENEWABLE ENERGY LABORATORY

2 – Approach (Technical)

Analysis interfaces with research and development

Rigorous Screening

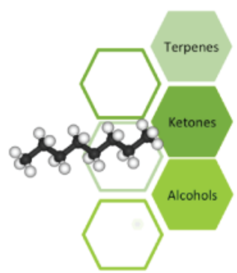
Rapidly identify viable candidates


Blendstock Evaluation

Measure properties

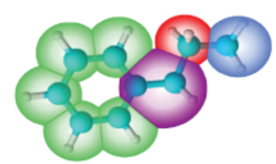
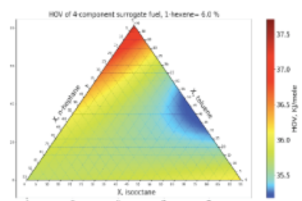
Populate database



Generate Insight

Develop blending models

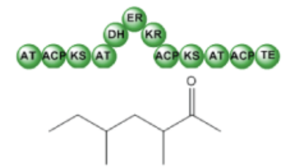
Correlate properties to molecular structure

Establish Bio Pathways

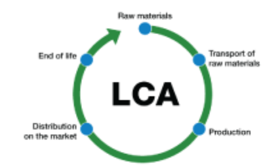
Target properties to generate key data

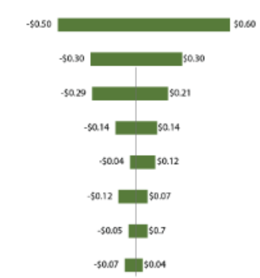
Conduct retrosynthetic analyses



Conduct Analyses

Provide improved data for LCA, TEA analyses

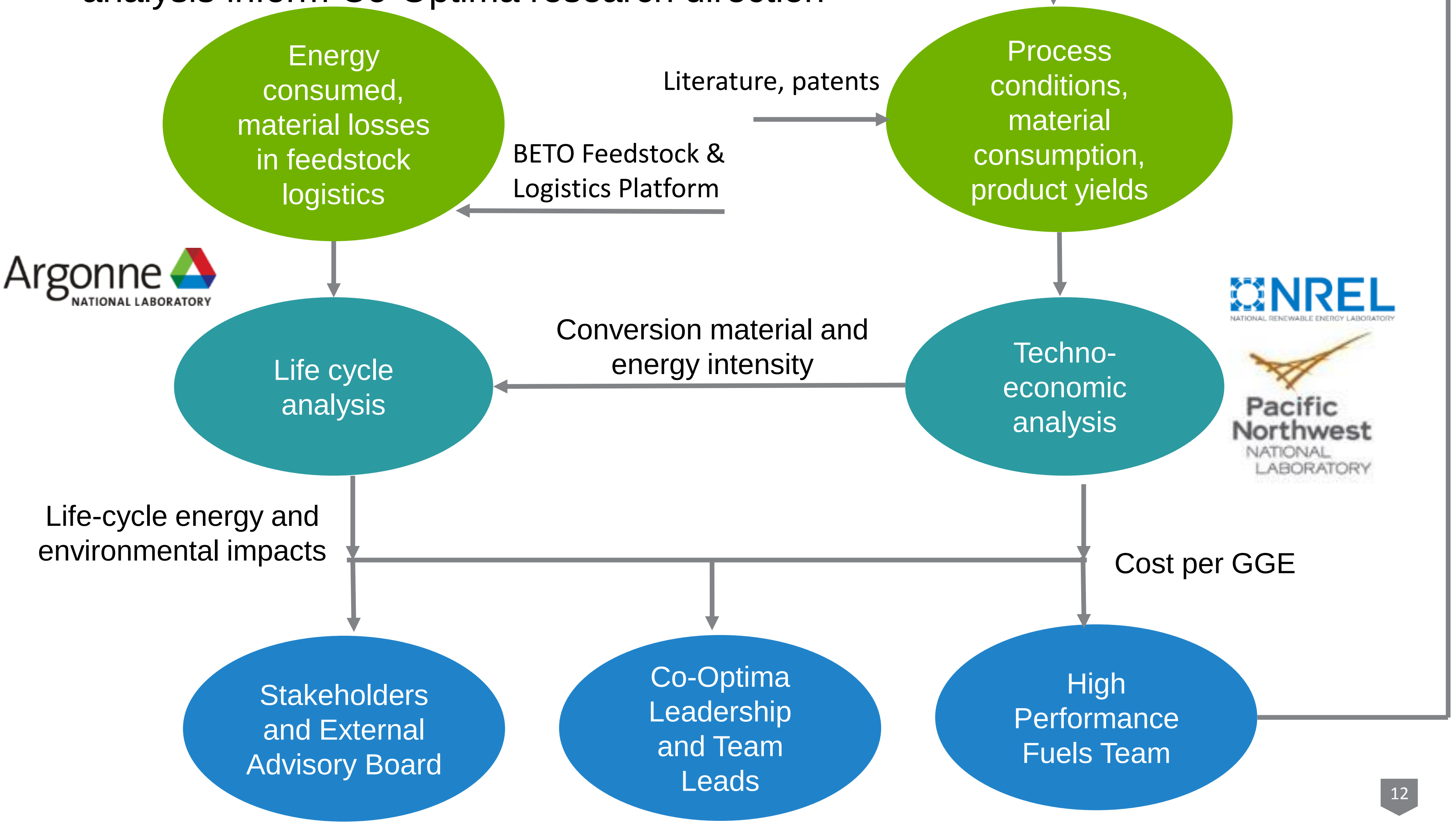




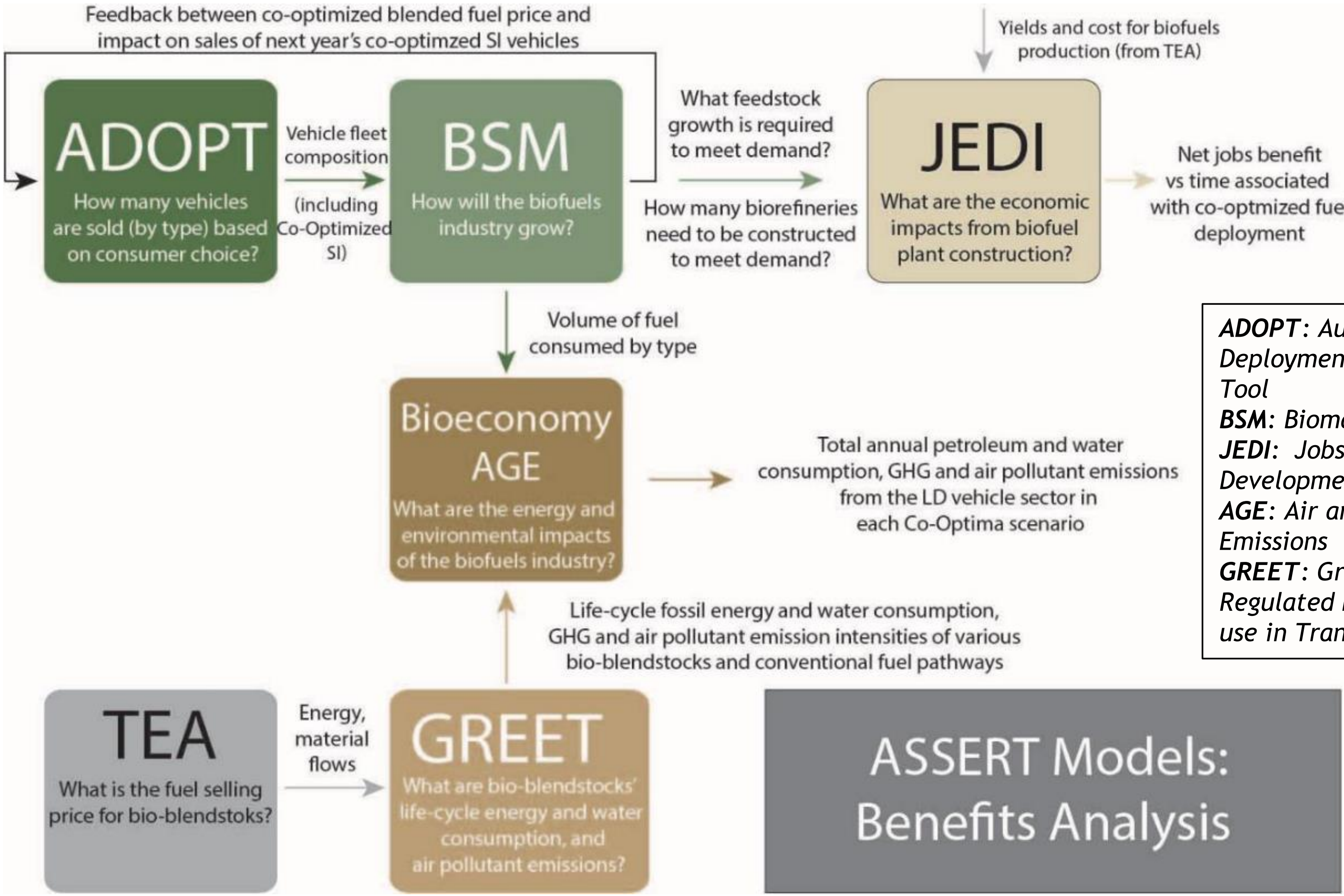
Gather input from technical teams, disseminate analysis results

Techno-economic and Life Cycle Analysis

Inter-linked techno-economic and life cycle analysis inform Co-Optima research direction



Benefits Analysis Technical Approach



ADOPT: *Automotive Deployment Options Projection Tool*
BSM: *Biomass Scenario Model*
JEDI: *Jobs and Economic Development Impact*
AGE: *Air and Greenhouse gas Emissions*
GREET: *Greenhouse gases, Regulated Emissions and Energy use in Transportation*

Estimating net job creation with JEDI

- Jobs are created at each stage in biorefinery infrastructure, on-going operation and the supply chains
- An input-output approach is used to estimate jobs supported by biorefinery construction and operation

Feedstock
Chemicals
Water/energy
Labor

→

→

Bio-blendstock

Co-products

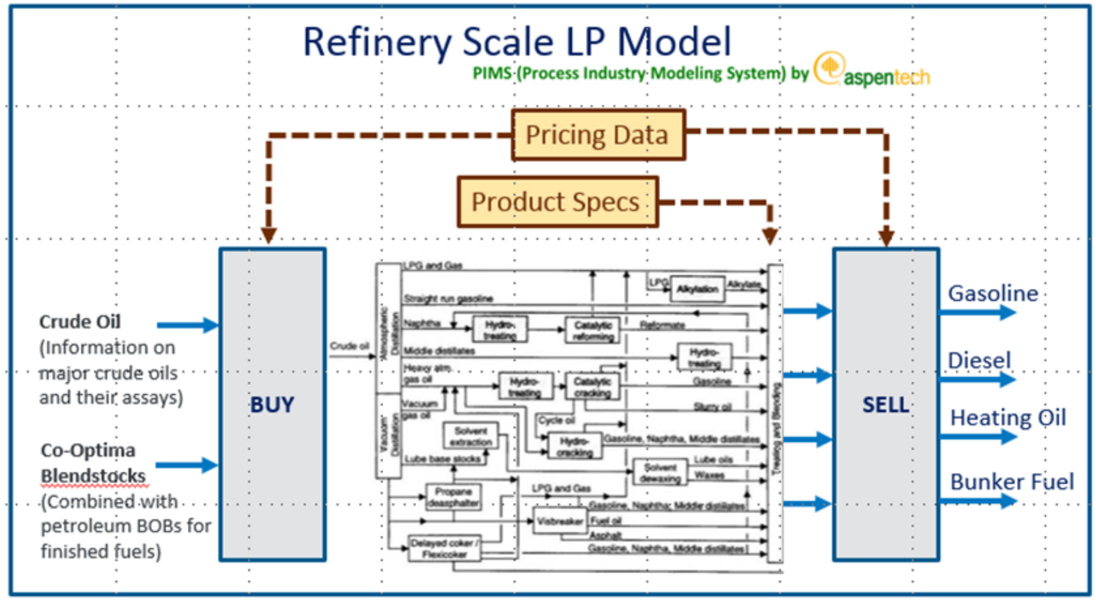
- Potential job substitution could occur in the petroleum industry
- Linear regression analysis is used to estimate the change in petroleum industry's employment

Changes in U.S. gasoline consumption → Changes in U.S. petroleum production → Changes in U.S. petroleum industry employment

Refinery Economics Approach

Modeled with Aspen PIMS

- Widely adopted software in fossil refining industry
- Primary petroleum processing units, capacities, and yield compositions are built in
- Allows analysis of production and blending of refinery streams to finished fuels



Inputs

- All major crude oils and property characteristics/assays reside in the existing PIMS database
- Detailed Co-Optima blendstock properties are added in

Methodology: Define objective function to maximize the refinery's profit margin subject to constraints: crude availability, process unit capacity limitations, and blending to meet final fuel specifications

Expert and literature resources

- Leverage technical expert insights from:
  - National laboratories
  - Original equipment manufacturers
  - Aftertreatment device manufacturers
  - Petroleum refiners
  - Non-profit organizations in the fuels and convenience store sectors
  - Regulatory agencies
  - Co-Optima External Advisory Board

- Build on information in the patent, peer-reviewed, and gray literature.

- Reduce uncertainty and define appropriate parameter ranges for sensitivity analyses

Milestones drive critical analyses

Task	Due	Description	Combustion Mode
B.4.1	1Q19	Define analysis approach (parameters, scenarios, methodology) for HD Benefits Bounding Analysis. Brief Extended Leadership Team and DOE to verify the analysis will address questions of Co-Optima leadership and team lead needs.	MCCI/KC
B.3.13	2Q19	Working with HPF, FP teams, select bio-blendstock candidates and provide list of 8-12 bio-blendstock candidates for consideration to COLT and DOE (MCCI)	MM/MCI
B.4.1	3Q19	COLT and DOE will be informed of the parameters, methodology, and results for feedback of heavy-duty bounding analysis through a report enabling them to provide feedback for analysis finalization.	MCCI/KC
B.3.13	4Q19	Complete screening of 8-12 bio-blendstocks so that the Co-Optima team is informed of their scalability and economic and environmental viability. Brief XLT, COLT, DOE on screening in a power point presentation. Results will be submitted to a journal in Q1 of FY20.	MM/MCCI
B.3.12	4Q20	B.3.12 Characterize impact (cost of ownership, GHG emissions, fuel consumption) of three strategies for co-design of fuels and engines for hybridized vehicles on individual vehicle level (in collaboration with other teams) and on a systems-level. Submit manuscript with analysis results.	BSI/MM
	4Q21	Integrate research and analysis outcomes of Co-Optima for the heavy-duty sector into 2-3 scenarios for co-optimized vehicle	MCCI/KC

Challenges and Critical Success Factors

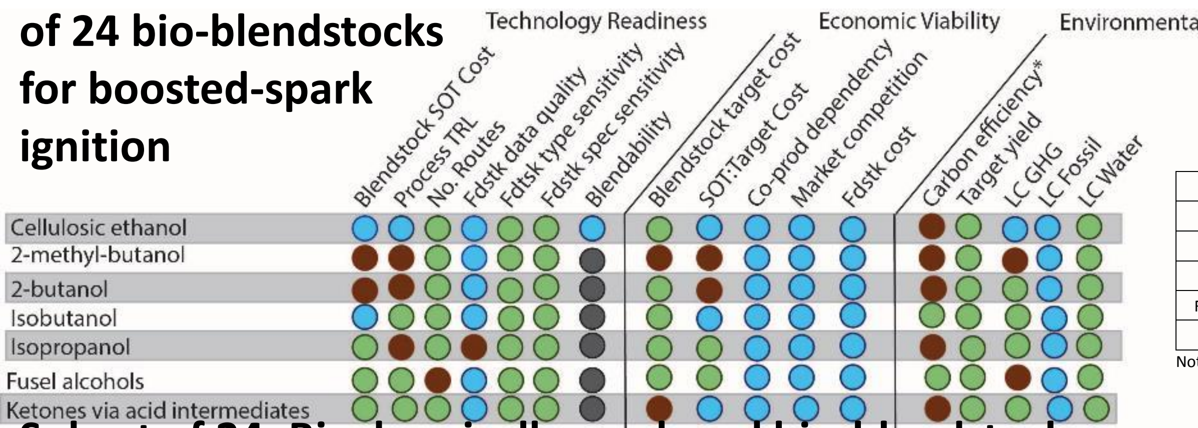
Challenges:
- Adequately characterizing technologies and systems ASSERT models
- Proprietary nature of early stage technology
- Managing data flow between models that are not explicitly linked

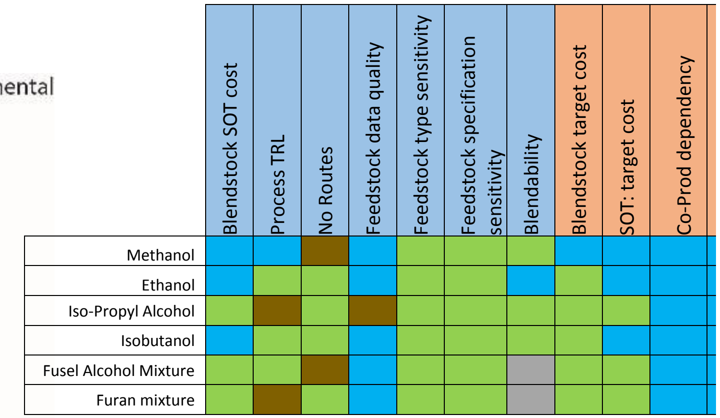
Critical Success Factors:
- Leveraging internal and external subject matter experts for insights into technologies and systems including bioprocessing, fuel distribution infrastructure, engine technology, aftertreatment device technology
- Seeking feedback regarding assumptions and scenarios used in ASSERT modeling from internal and external experts
- Regular communication among team members, careful and collaborative review of each model's input and output

3- Technical Accomplishments

Economic, environmental, and scalability evaluation of bio-blendstocks

Economic, Environmental and Scalability Screening of 24 bio-blendstocks for boosted-spark ignition

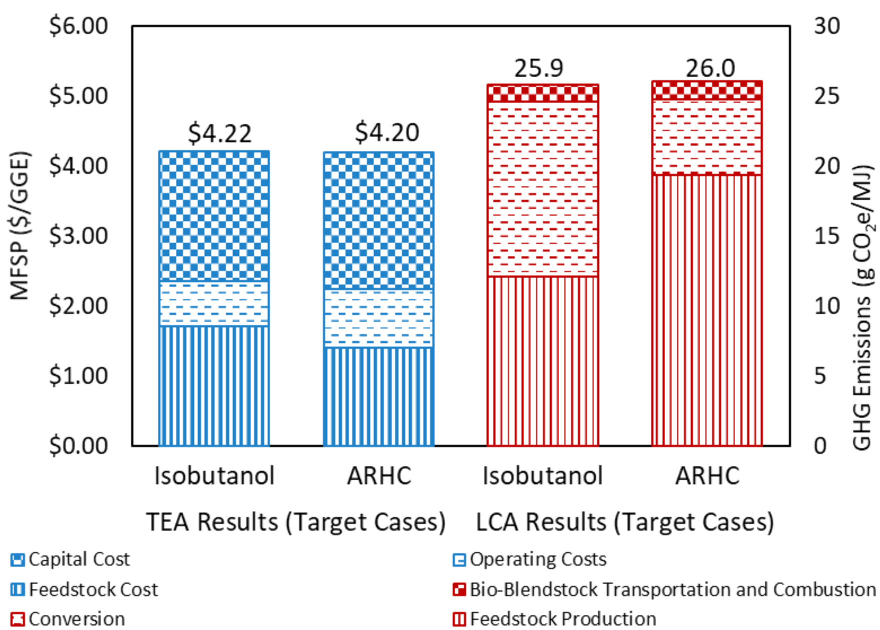




Note 1: Blue, green, and Brown boxes represent favorable, neutral, and unfavorable categorization

Subset of 24: Biochemically produced bio-blendstocks

Blue: Favorable, Green: Neutral, Brown: Unfavorable, Gray: Inconclusive

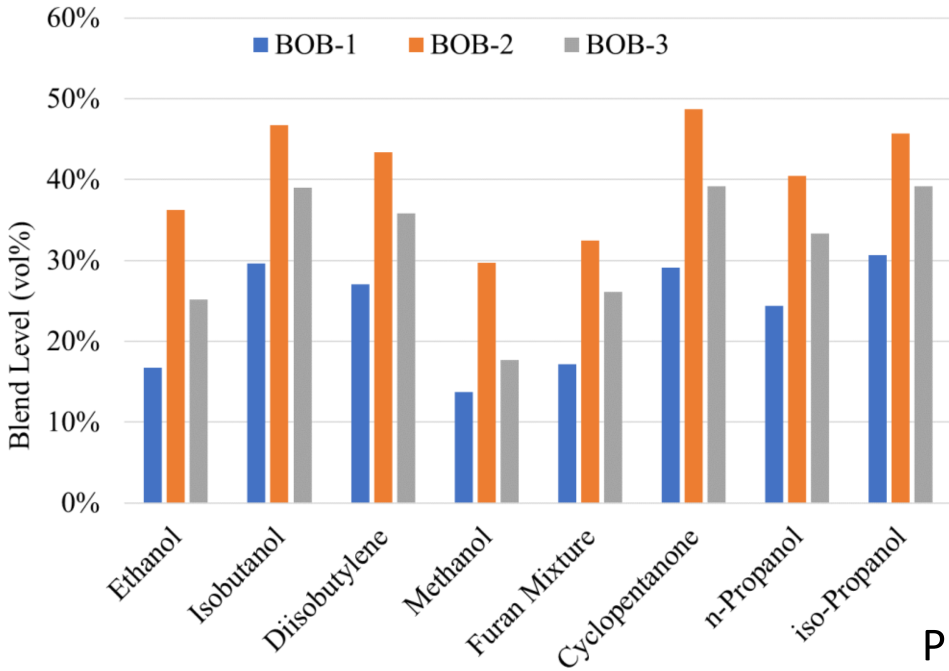


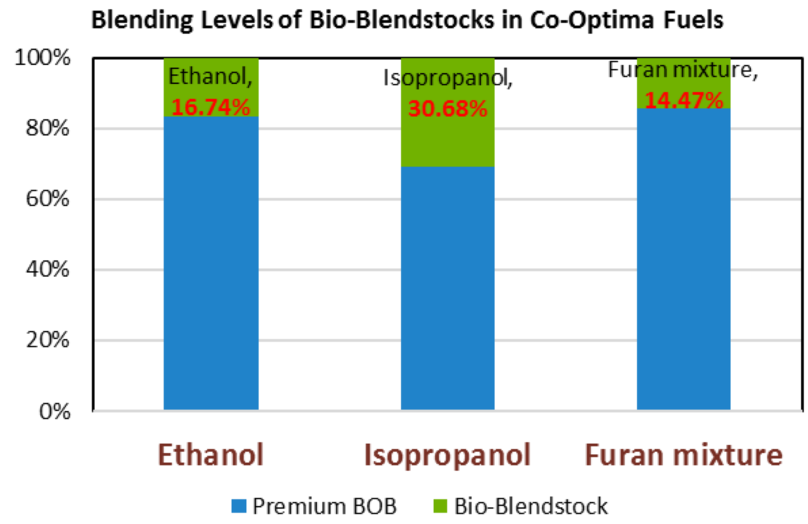
Contribution to Co-Optima Top Ten Bio-Blendstocks report

Detailed TEA and LCA of bio-blendstocks

ARHC: Aromatic-rich hydrocarbons

Bio-blendstock selection for benefits analysis



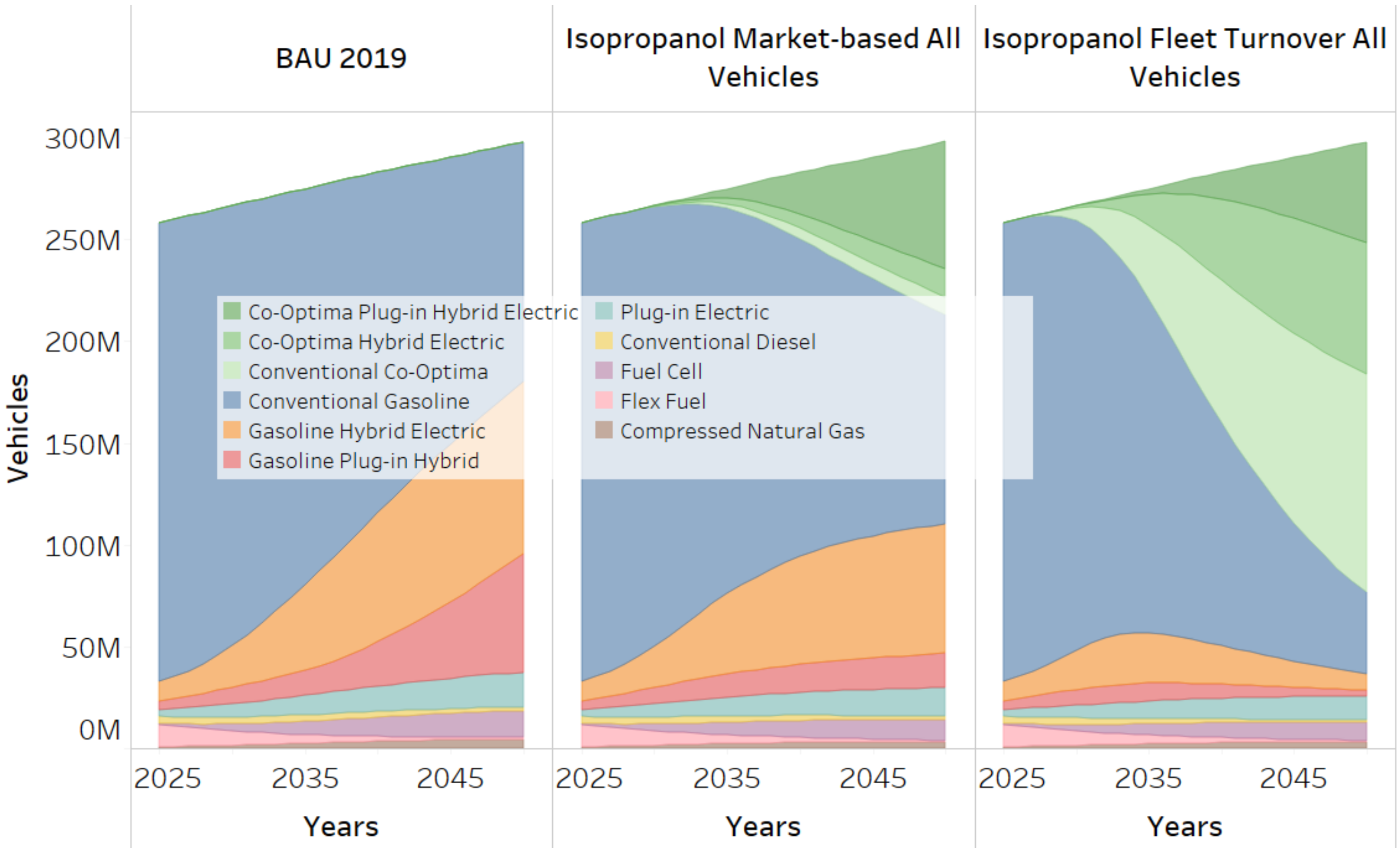


Preliminary results shown for isobutanol cases

Collaboration with Fuel Properties team to use merit function for identification of bio-blendstocks that can achieve 10% engine efficiency gain relative to E10 at lower blending levels.

Note: furan mixture is 60% 2-methylfuran, 40% 2,5-dimethylfuran mix

Fleet composition shifts as vehicles with co-optimized engines become available

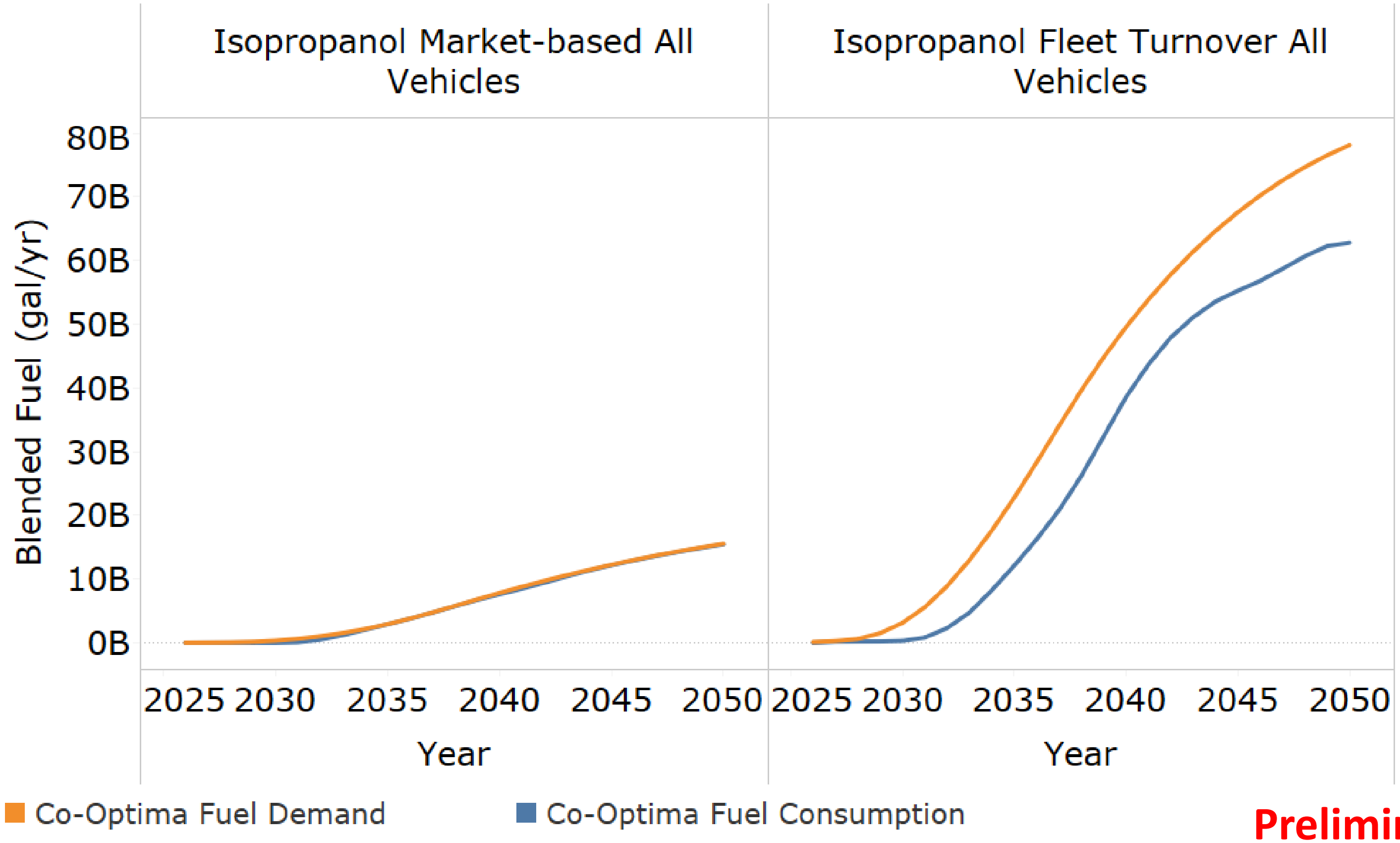


- Analyses explore potential influence of Co-Optima on hybridized vehicles
- Upper bound scenarios affect all vehicles

Preliminary Results

- ADOPT models the light-duty fleet comprehensively including many different vehicle technologies
- Adoption of vehicles with co-optimized engines is influenced by pace of biorefinery build-out in BSM, among other factors

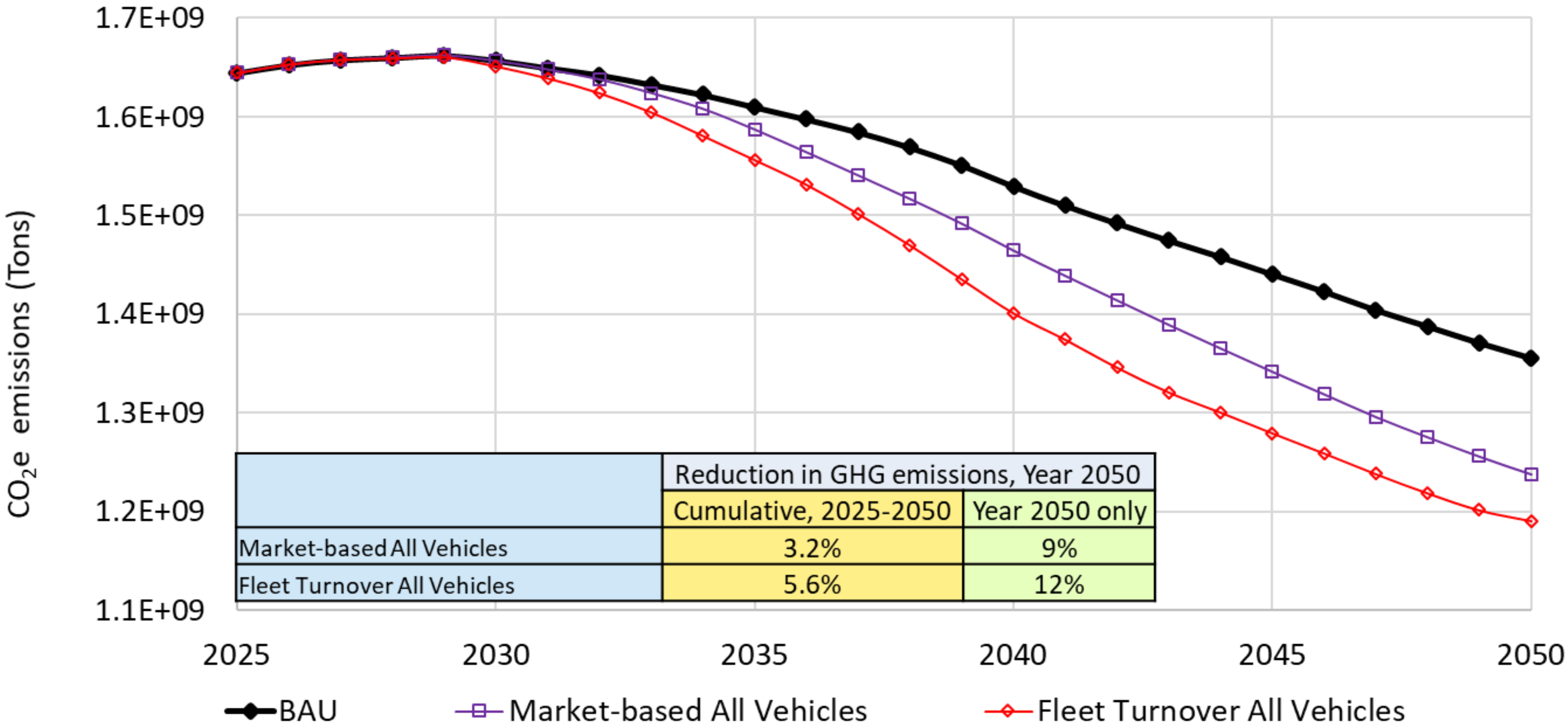
Bio-blendstock production reaches 16 billion gal



Preliminary Results

- Investment in nascent technologies may be limited in part because of the high expected return on investment
- Bio-blendstock availability affected by feedstock scarcity, limits in biorefinery expansion to meet demand, and limitations in compatible dispensers
- BSM logic updated to include latest thinking on biomass-based hydrocarbon infrastructure costs and needs

Annual GHG emissions reductions could reach 12% in 2050 as upper bound



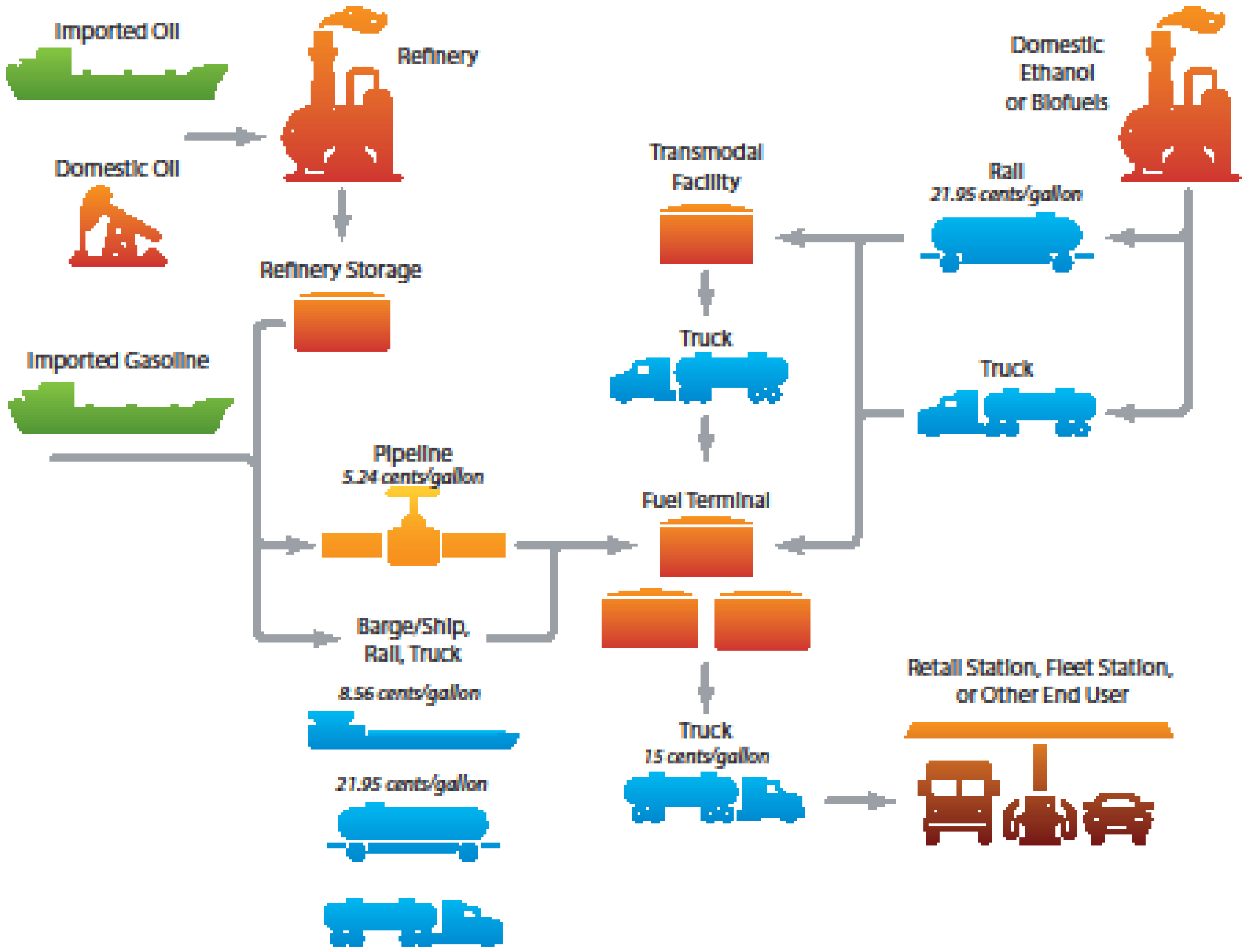
	Reduction in GHG emissions, Year 2050	
	Cumulative, 2025-2050	Year 2050 only
Market-based All Vehicles	3.2%	9%
Fleet Turnover All Vehicles	5.6%	12%

Preliminary Results

- Technology takes some time to impact the fleet as it is introduced
- Significant reductions in GHG emissions to be expected in out years
- Ongoing work investigates these dynamics and considers furan mix, E17, limiting technology expansion to internal combustion engine vehicles

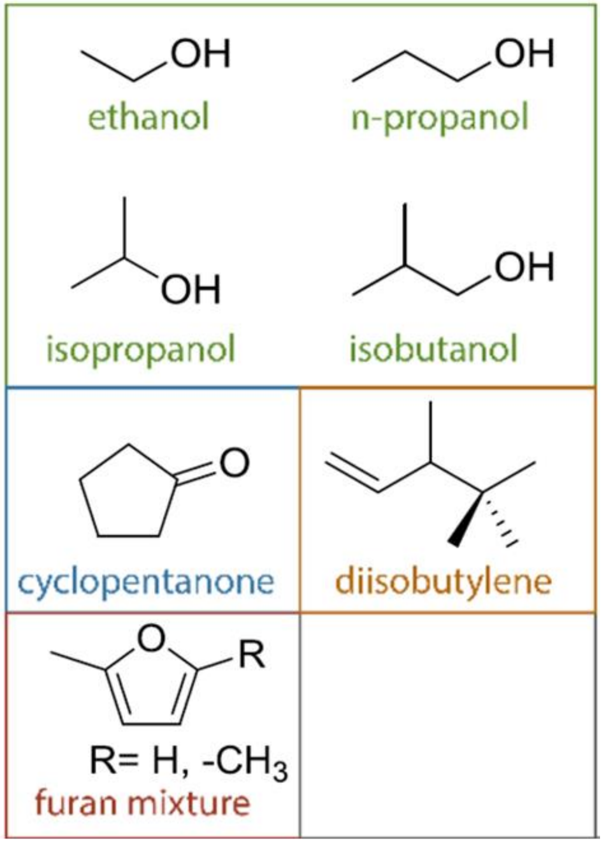
Infrastructure costs estimated for distribution segments by fuel type

- Fuels with properties similar to conventional fuels with adequate research could travel via pipeline
- Fuels with properties dissimilar to conventional fuels would likely travel by rail and barge



Technical Approach: Refinery Economic Analysis

OBJECTIVE: For seven Co-Optima bio-based blendstocks with desired fuel properties, characterize the potential economic value to petroleum refiners.



Methods:

- Used pure and blended property experimental data from the Fuel Properties and High Performance Fuel teams
- Modeled with Aspen PIMS optimization and refinery planning software

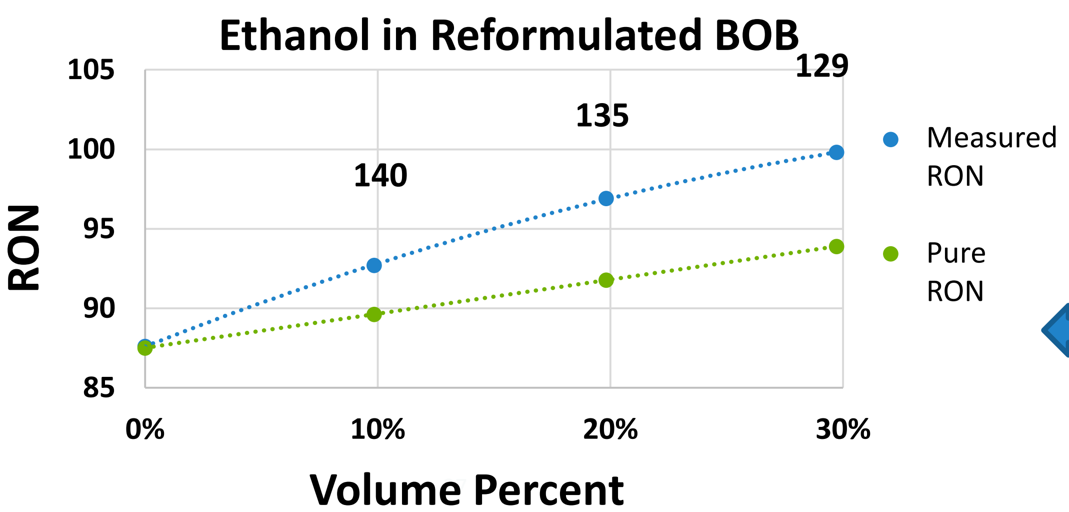
Analysis Included in Report:

1. ***Octane Impacts:*** Co-Optima Blendstocks compared with Petroleum Reformate
2. ***RVP and Octane Impacts:*** Blending with Select Refinery Streams
3. ***Meeting Fuel Specs:*** Evaluation of Representative Refinery Performance
4. ***Meeting Fuel Specs:*** Individual Refinery-by-Refinery Blending
5. ***Summary, Conclusions, Next Steps***

Co-Optima Blendstocks compared with Reformate

Adopted data from fuel proprieties team measurements
including pure and blending octane numbers

Bio-blendstock	Pure Component RON	Blending RON @ 10 vol.%	Blending RON @ 20 vol.%	Blending RON @ 30 vol.%	Effective RON (Average)
Ethanol	109	140	135	129	134.6
i-Propanol	113	119	122	122	121.0
n-Propanol	104	122	122	118	120.6
i-Butanol	105	113	113	114	113.3
Diisobutylene	106	117	119	118	118.0
Cyclopentanone	101	114	119	116	116.3
Furans	112	146	134	124	134.6

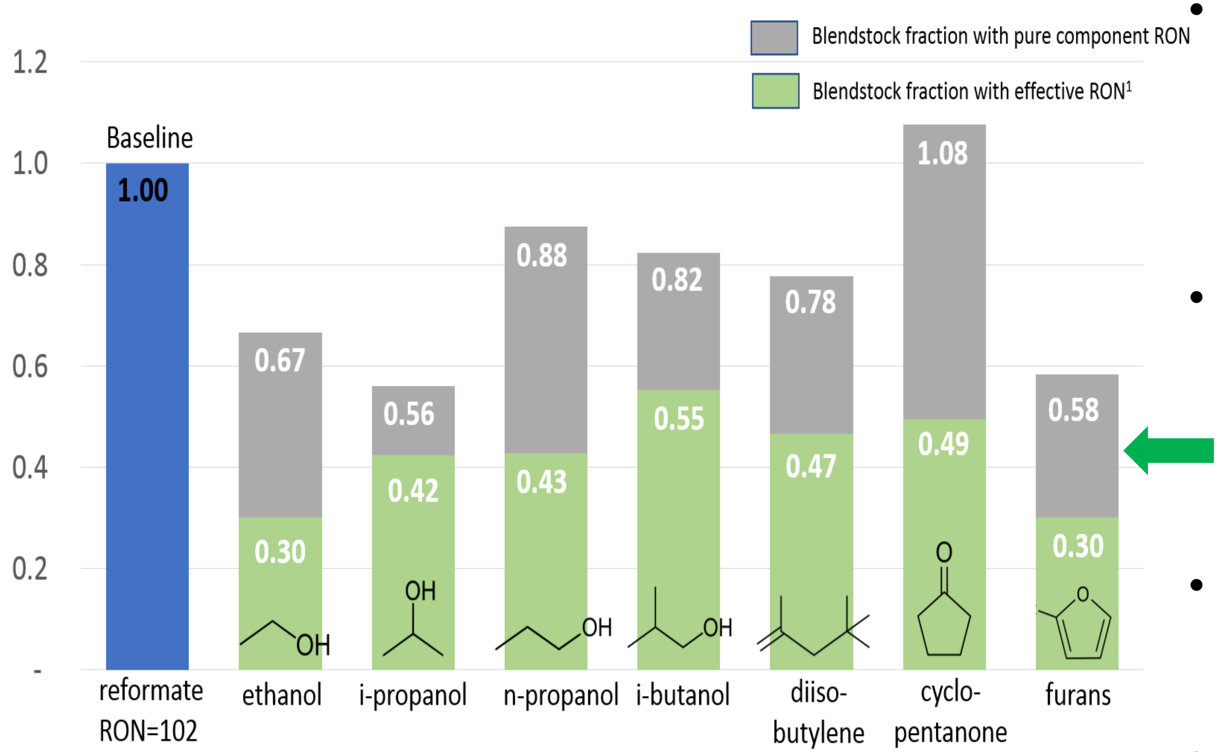


Based on experimental results:

- Co-Optima bio-blendstocks exhibited synergistic non-linear behavior when blended with traditional hydrocarbons.
- These **oxygenated Co-Optima blendstocks had a significantly higher blended RON** than would be predicted by linear pure component blending.

Refinery Economics: Examination of Octane Impacts

Co-Optima Blendstocks compared with Reformate

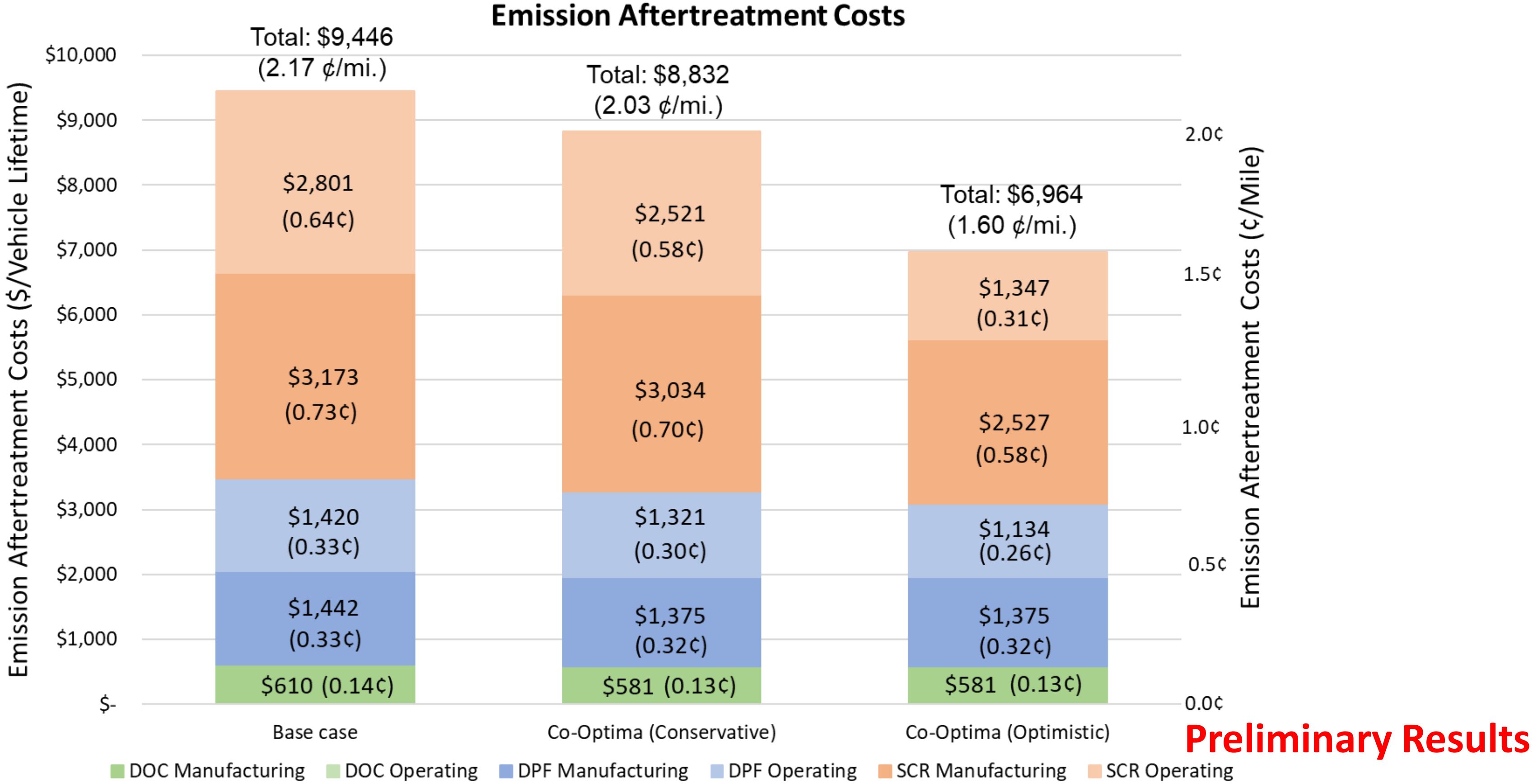


Blendstock volumes required to produce 95 RON fuel from 88 RON BOB, based on pure component RON and effective RON, relative to reformate with 102 RON

RESULTS

- **IDENTIFIED 7 MOLECULES/ MIXTURES** enabling non-linear synergistic blending behavior with petroleum hydrocarbons
- **LOWER BLEND VOLUMES** needed for 6 out of the 7 to convert 88 RON BOB to 95 RON fuel relative to petroleum reformate
- **BENEFIT** of octane number boost depends on initial BOB octane
- **OTHER PROPERTIES** such as RVP, octane sensitivity, drivability index also considered

Co-Optimizing fuels and MCCI engines could reduce emissions and aftertreatment device costs



- We explored the range in potential aftertreatment device capital and operating cost savings through co-optimization of MCCI engines and fuels with a new modeling tool
- Smaller diesel oxidation catalyst (DOC), diesel particulate filter (DPF), and selective catalytic reduction (SCR) devices saves capital costs
- SCR urea use decreases when engine-out NO_x emissions are lower
- DPF regeneration is less frequent and consumes less diesel fuel when engine-out PM emissions are lower

4 – Relevance

ASSERT evaluates the bio-blendstocks and engine technologies under consideration within the Co-Optima program from an environmental and economic perspective while conducting research and development-guiding analyses.

Relevance to MYPP Barriers

MYPP Barrier	ASSERT approach to addressing
Co-development of fuels and engines has the potential t o increase vehicle engine efficiency, improve fuel eco- nomy, and reduce emissions [ADO-E]	Quantification of economic, environmental, and employment benefits or drawbacks helps BETO evaluate benefit of program and communicate to stakeholders.
Knowledge of the influence of bio-intermediates blending with petroleum processing is still in the developmental stage [ADO-G]	The value to the petroleum refiner for blending Co-Optima fuels with refinery fuel blend components is estimated with methods used by the petroleum industry allowing further understanding of which blends are likely to have the largest impact.
Analysis is needed to better understand factors influen- cing the growth and development of the bioenergy and bioproducts industries, identify the most impactful R&D strategies [At-A]	Biorefinery expansion modeling with the BSM improves understanding of which factors influence the growth and development of the biofuels industry.
High-quality analytical tools and models are needed to better understand bioenergy supply chain systems, link- ages, and dependencies. Models need to be developed and refined to reflect new knowledge, scientific break- throughs, and enable informed decision-making. Improvements in model components and linkages are necessary to improve utility, consistency, and reliability. [At-B]	The ASSERT team works to improve characterization of the supply chain and risk into key models, update all models to reflect currently available data, and applies analysis results to setting of technical targets and programmatic goals.

4 - Relevance

How ASSERT efforts impact the BETO program

VTO Program Interactions

- Engine Research
- Fuels and Lubricants
- Electrification

Requirements

- BETO MYPP
- Co-Optima Advanced Engine Development
- Co-Optima Fuel Properties
- EAB
- Stakeholders

Co-Optima

- Analysis
- Blendstock Generation
- Fuel Property Characterization
- Structure-Property Relationships

BETO Program Interactions

- Analysis and Sustainability
- BETO Core Conversion
- ChemCatBio
- Separations Consortium
- Agile Biofoundry
- Feedstock-Conversion Interface Consortium

Data and Outputs

- Fuel Property Database
- Bio-blendstock Screening
- Benefits, Refinery Integration, Techno-economic, Lifecycle Analyses
- Co-Optimizer

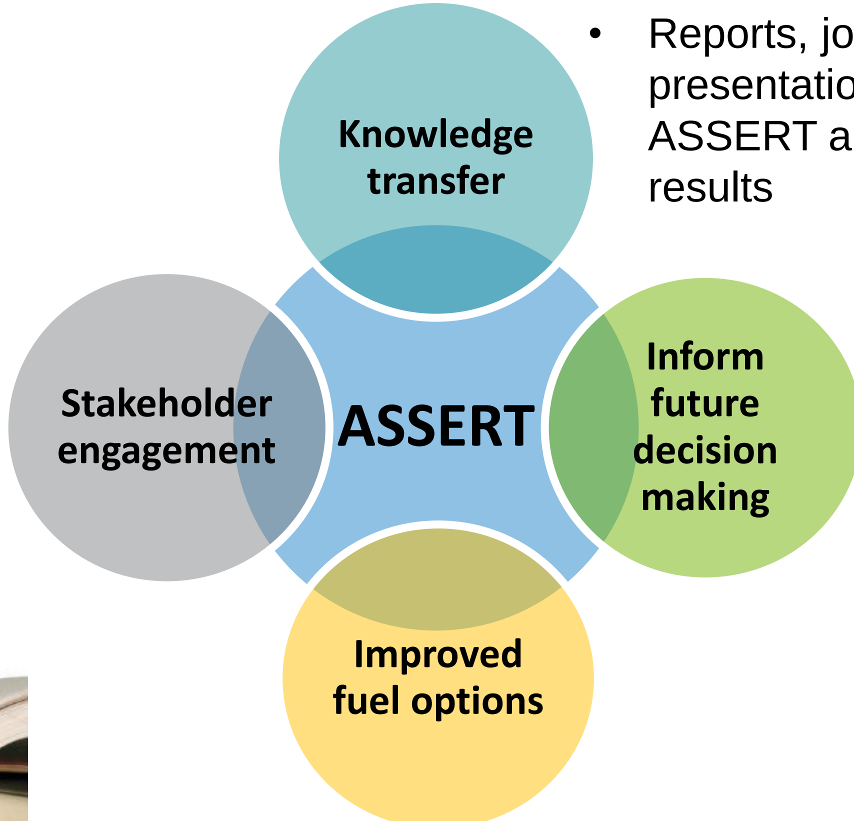
Provide additional insights into costs and sustainability of biofuel production, adoption that other BETO programs can leverage

Relevance to other BETO projects

- Close link to BETO's Analysis and Sustainability platform through use of models developed under that platform including JEDI, GREET, refinery modeling, and BSM.
- Ongoing work with conversion platform to share analysis results and key lessons learned when considering a wide range of fuel products.
- Further, analysis methodology to assess benefits of Co-Optima can be applied in other projects as can improvements, refinements, and expansions of the ASSERT suite of models.
- Insights ASSERT gains into barriers to large-scale deployment of co-optimized fuels and engines can inform BETO research and development priorities and directions overall.

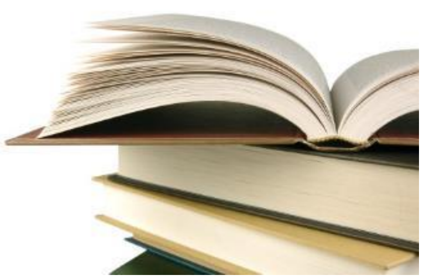
Relevance to Bioenergy Industry

- Deep dive presentations on stakeholder calls
- TEA/LCA tutorial for university teams
- Work with EAB to provide guidance on the direction of ASSERT analyses and feedback on results



- Reports, journal articles, presentations documenting ASSERT analyses and results

- Provide insights into potential influence of bio-blendstocks on jobs
- Disseminate information on scalability, economic viability, and environmental sustainability of bio-blendstocks that may be of interest to industry
- Outline key economic and sustainability drivers and barriers for moving fuels to market



Investigate a range of fleet options

- Light duty
- Medium duty
- Heavy duty

5 – Future Work

Economic, environmental, and scalability evaluation of MM and MCCI bio-blendstocks

Milestone: Evaluate between 8 and 12 bio-blendstocks in FY19 to provide insight into the viability of potential MCCI and MM bio-blendstocks (FY19, Q4)

Metric	Favor-able	Neutral	Unfavorable	Approach
Technology Readiness: Process modeling data source	Demo scale	Bench scale	Partly literature based	Conduct review of existing research and analyses, literature, and discussions with national laboratory researchers.
Economic Viability: Cost reduction needed to go from SOT to target case	<2	2-4	> 4	Based on ratio of Min Fuel Selling Price of state of technology (SOT) case to target case.
Environmental Sustainability: Carbon efficiency; fossil and renewable input carbon (target case)	>40%	30%-40%	<30%	Based on known conversion methods and input from HPF team & lit, how would the candidate be made? Use high- level TEA mass balance to estimate

EXAMPLE metrics of 17 total.

In FY18, ASSERT revised the analysis metrics covering economic, environmental, and technology readiness factors used in FY16-18 for BSI blendstocks. We evaluated 3 MCCI bio-blendstocks.

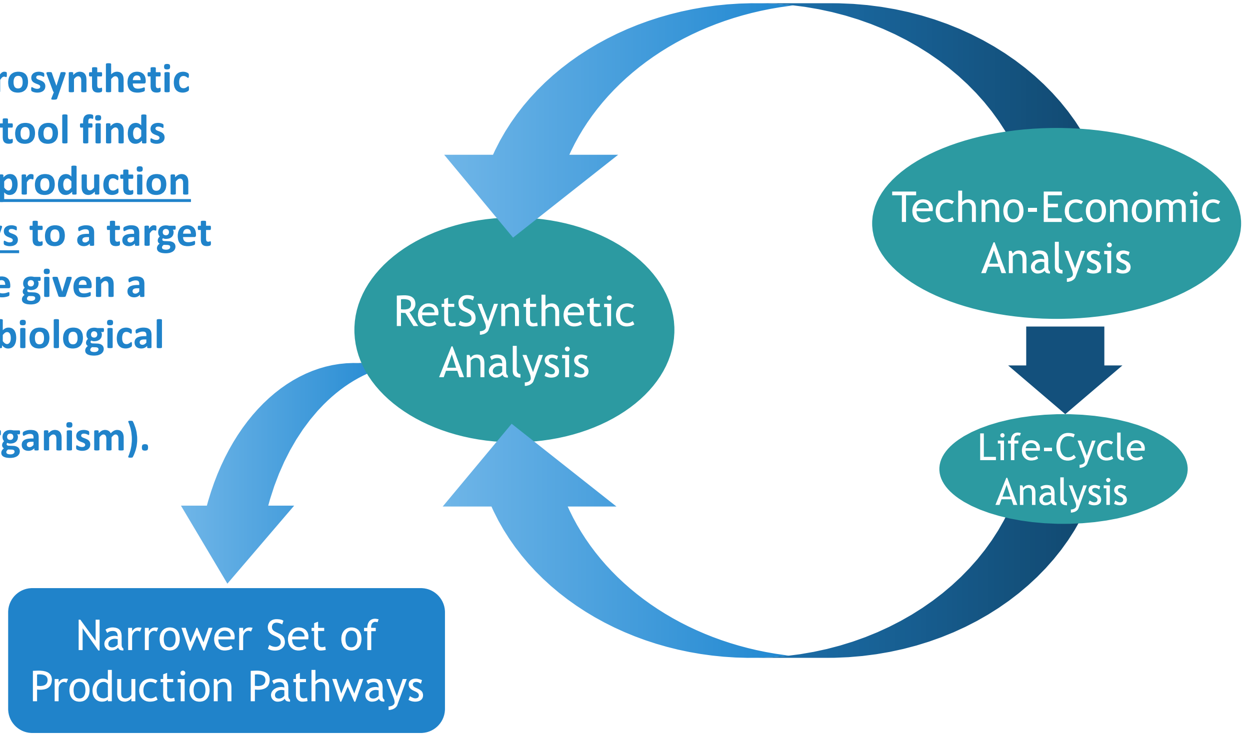
We will apply these metrics to the evaluation of additional MM and MCCI bio-blendstocks.

We are coordinating with HPF and FP teams to select bio-blendstocks.

Integration of TEA and LCA into retrosynthetic analysis

- The HPF team has developed and continues to refine and apply a retrosynthetic analysis tool
- In FY19, ASSERT is exploring whether it is possible to incorporate elements of techno-economic and life cycle analyses into this tool to narrow down pathway options with economic and sustainability considerations
- The objective of this task is to maximize utility of tools produced in the Co-Optima portfolio
- During FY19, ASSERT will determine whether this type of incorporation is feasible, only developing an approach if it would be defensible and yield reliable insights

The restrosynthetic analysis tool finds <u>optimal production pathways</u> to a target molecule given a starting biological chassis (microorganism).



Incorporation of techno-economic and life cycle analyses into the tool could narrow pathway choices based on ease of processing and sustainability factors

Strategic R&D Guidance for Co-Deployment of Hybridized and Co-Optimized Vehicles

Motivation: Understand the implications of hybridization on fuel/engine requirements to maximize commercial relevance and impact of co-optimized fuels.

Sample key questions: What will be the impacts of increasing hybridization on ICE engine requirements? What are the practical efficiency gains co-optimized fuels and engines, tailored to work in HEVs and PHEVs, could achieve?

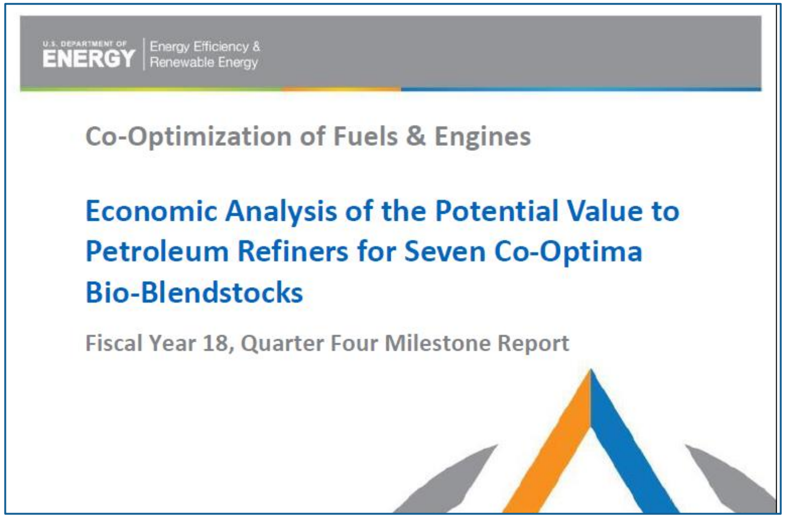
Outcomes:

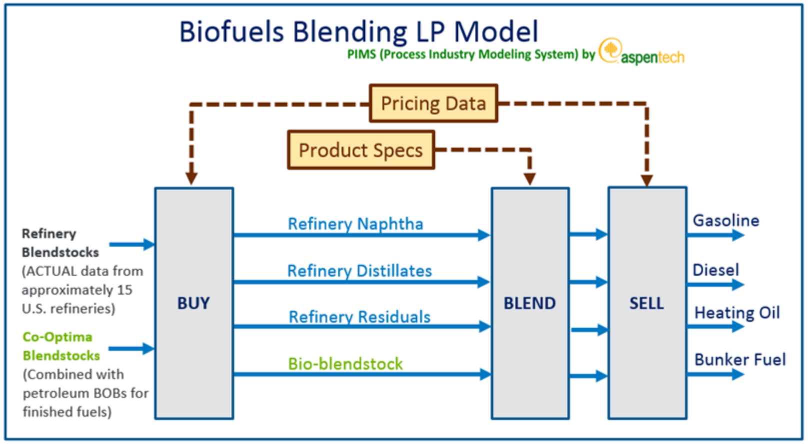
- Inform development of research portfolio that takes into account the expanding role of hybridization
- Establishment of technical targets such as engine efficiency metrics.

Milestone: Characterize impact (cost of ownership, GHG emissions, fuel consumption) of three strategies for co-design of fuels and engines for hybridized vehicles (FY20, Q4)

Refinery Economics Next Steps

- External review prior to FY18 report release
- Build on learnings and tools from Boosted-SI studies (e.g. Aspen PIMS, conversion models) for select Co-Optima light, medium, heavy duty and multi-mode bio-blendstocks not considered in FY18
- Work with data from the Fuel Properties and High Performance Fuel teams and identify data gaps
- Incorporate sustainability drivers in our analysis as part of our FY19 work plans





Outreach to university partners on TEA and LCA

- Analysis, including TEA and LCA, is a mandatory part of the university projects that were awarded through a BETO Funding Opportunity
- ASSERT will enable consistent analysis techniques within the university projects such that analysis results across the Co-Optima program are comparable.
- ASSERT will kick off interactions with university teams with a tutorial in techno-economic and life-cycle analysis
- The tutorial will increase students' knowledge regarding TEA and LCA and move the university teams towards adopting consistent approaches and assumptions with the ASSERT team for results comparison

5 - Summary

Summary

Overview	Evaluate the blendstock and vehicle technologies under consideration within the Co-Optima program from environmental and economic perspectives while conducting research and development-guiding analyses.
Approach	• Techno-economic and life-cycle analysis, high-level and detailed • Benefits analysis with modeling suite covering vehicles, biorefineries, jobs, and environmental effects • Refinery economic analysis • Bounding analyses to bookend potential benefits of co-optimization approaches
Technical Progress	• **Bio-blendstock screening-** Screened 24 BSI bio-blendstocks, 3 MCCI bio-blendstocks for economic, environmental, and scalability viability • **Benefits characterization -** Quantified potential energy, GHG, water, air pollutant benefits to deployment of co-optimized fuels and BSI engines • **Quantified value to refiners, heavy-duty vehicle manufacturers -** Refinery economics and MCCI value proposition tasks guide Co-Optima R&D towards industry-relevance, impact
Relevance	**Enhance bioenergy value proposition by identifying scalable, economically viable bioblendstocks that maximize engine performance and energy efficiency, & minimize environmental impacts**
Future Work	• Screen MM and MCCI bio-blendstock candidates • Evaluate refinery economics for MM and MCCI bio-blendstocks • Characterize opportunity space for co-deployment of co-optimized and hybridized vehicles to inform Co-Optima R&D plans