

DOE Peer Review Conversion R&D

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Kevin Craig

Conversion R&D Program Manager

kevin.craig@ee.doe.gov

303-434-6899

Conversion R&D Team – DOE and Fellows

DOE Staff

Dr. Ian Rowe

Beau Hoffman

Dr. Gayle Bentley

Dr. Sonia Hammache

Trevor Smith

Liz Moore*

Andrea Bailey*

AAAS Fellow

Dr. Joel Sarapas

DOE Scholar

Ross Houston

Kevin Craig, Program Manager



Ian



Beau



Sonia



Gayle



Trevor



Andrea



Liz



Joel



Ross

Conversion R&D Team –Contractor Team

Conversion Support Contractors

Jessica Phillips - BGS, Manager

Mark Philbrick – BGS

Chidiebere Agwu - BGS

Ben Simon - BGS

Mary Kate O’Brien - BGS

Jesse Glover - BGS

Seth Menter – BGS

Robert Natelson – BGS

Brittany Clark – The Building People, LLC



Jessica



Mark



Chidiebere Agwu



Jesse



Robert



Seth



Mary Kate



Brittany



Ben

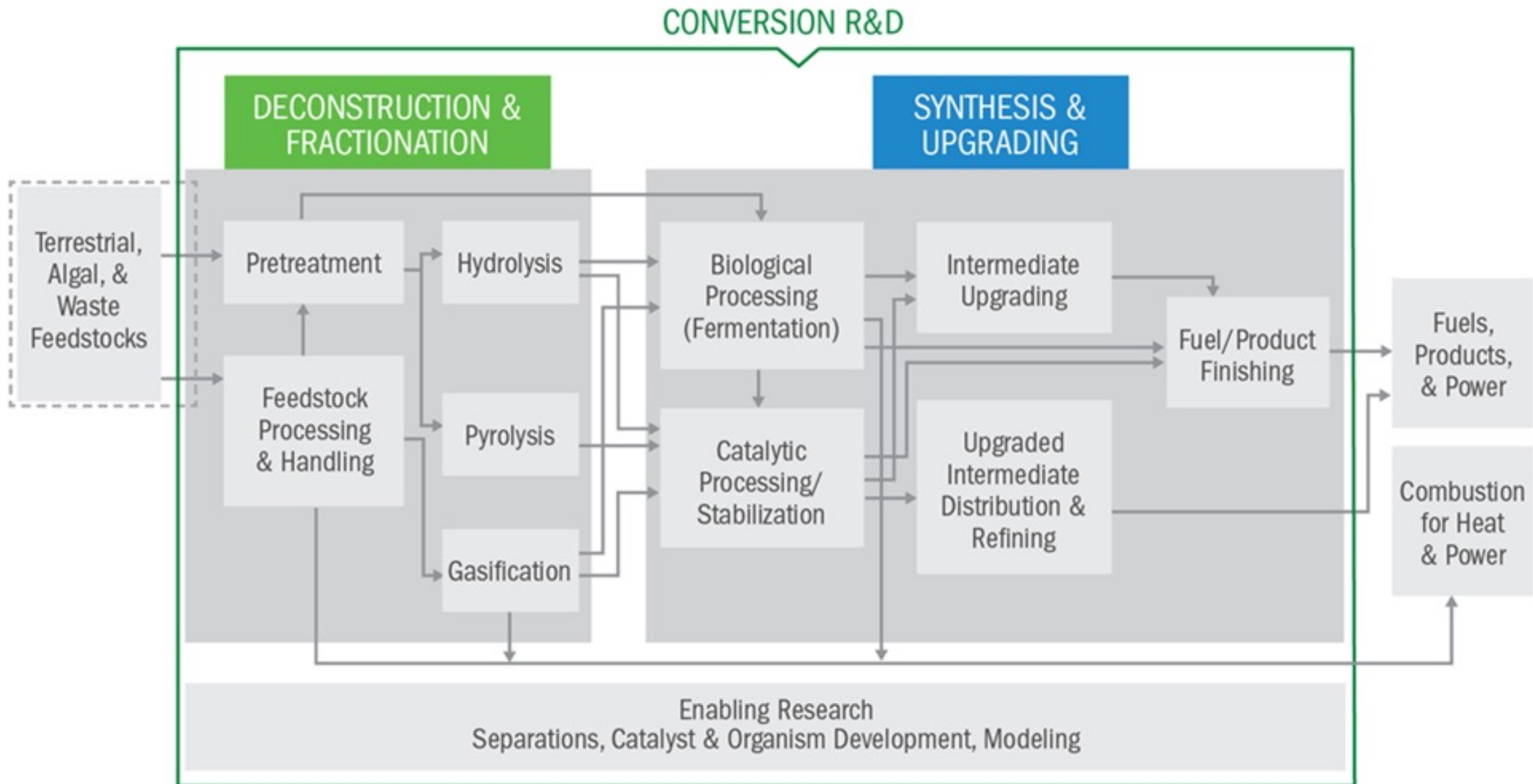
Program Goals – Conversion R&D

- Strategic Goal
 - The strategic goal of the Conversion R&D program is to develop efficient and economical biological and chemical technologies to convert biomass feedstocks into energy-dense liquid transportation fuels, such as renewable gasoline, diesel, and sustainable aviation fuel (SAF), as well as bioproducts, chemical intermediates
- Performance Goal
 - By 2021, complete the research necessary to enable an integrated technology pathway verification at engineering scale in 2022 of a process that yields a mature modeled MFSP of \$3/GGE or less for production of a hydrocarbon biofuel and, where appropriate, a coproduct, and which has a minimum 60% reduction in GHG emissions relative to currently predominant fuel.

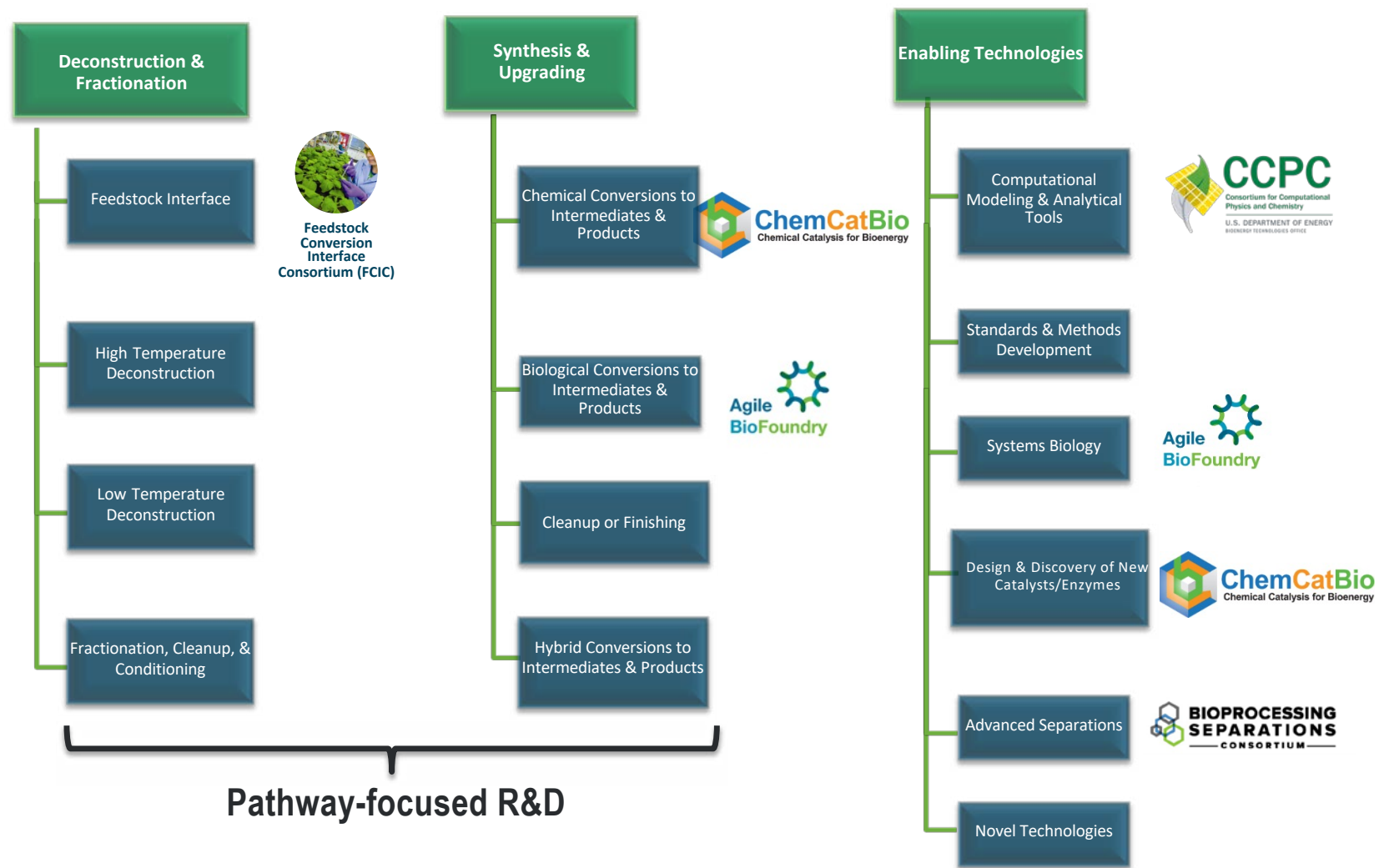
Conversion R&D Performance Goals (2020 MYP update)

- By 2022, achieve 90% monomeric sugar yield from hydrolysis of deacetylation and mechanical refining (DMR) solids at low (10 milligrams/gram) protein loading using a new DMR-specific enzyme cocktail formulation.
- By 2023, demonstrate an integrated lignin valorization process that achieves 60% carbon valorization of real lignin from a hardwood, grass, or agricultural residue. Instead of being a cost burden from a capital and operating cost perspective, this lignin valorization process will reduce the MFSP by at least \$0.25/GGE.
- By 2024, complete the R&D necessary to define a route to a 2030 verification of a mature modeled MFSP of \$2.5/GGE or less for biomass through a conversion pathway to hydrocarbon biofuel and coproducts with a GHG emissions reduction of 60% or more compared to currently predominant fuel.
- By 2025, produce bioproducts at needed scales (20–100 kilograms) for product testing to support off-take agreements and end-user/market acceptance.
- By 2026, demonstrate at least three fully integrated bench-scale processes that employ catalysis (biological and/or chemical) that are able to upcycle at least three large-market commodity polymer materials to higher-value materials that meet the 2-times economic incentive, greater than 50% energy savings relative to virgin material production, and retain at least 75% of the carbon present in the original polymer in the upcycled product. Demonstrate these fully integrated processes on both clean and realistic plastics streams, the latter as would be encountered after separations at a materials recovery facility

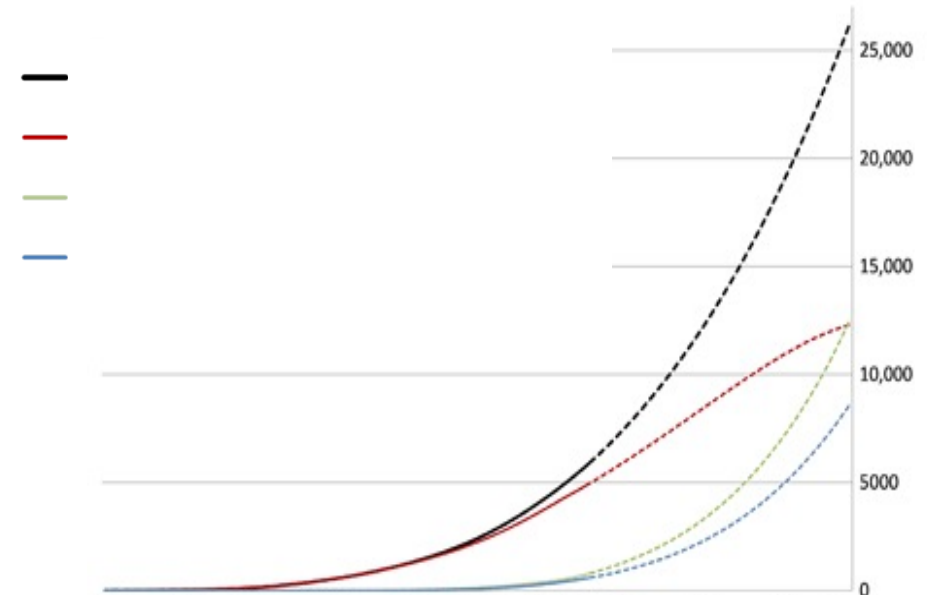
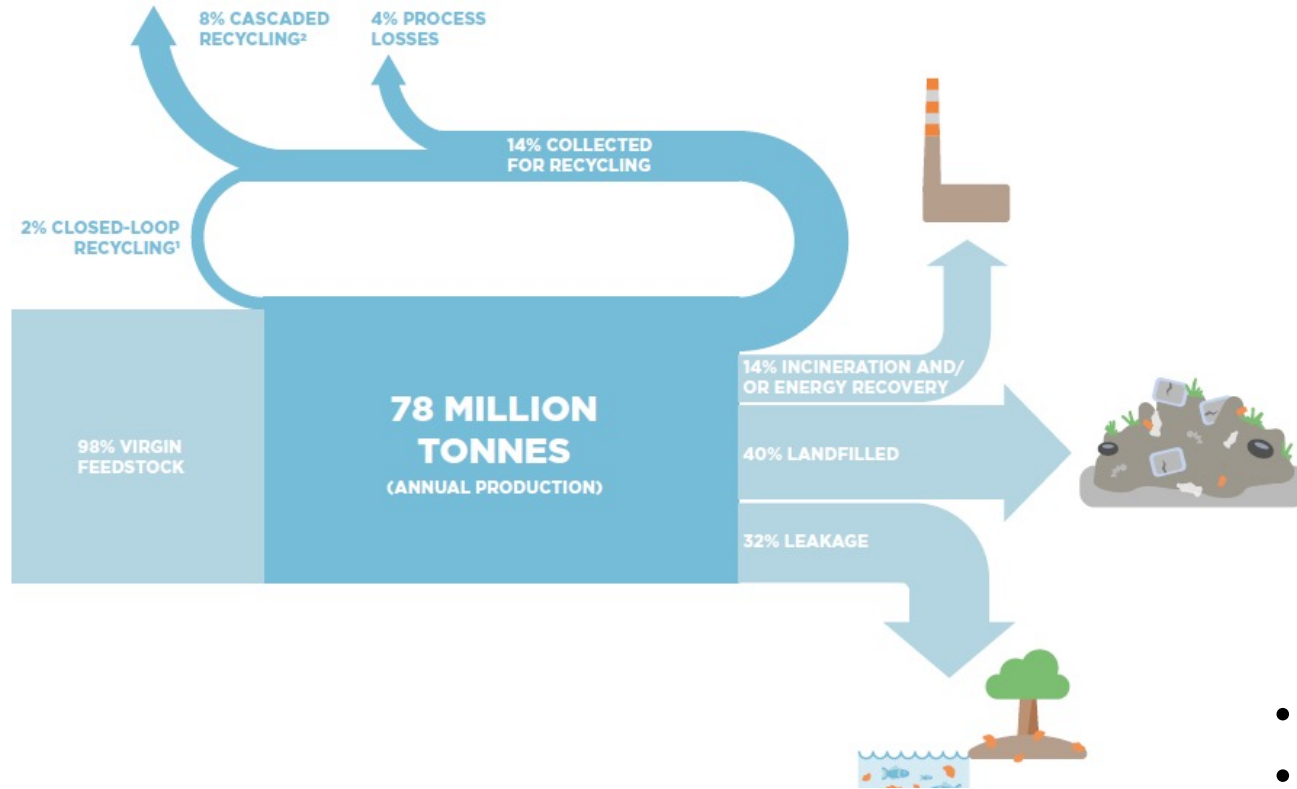
Program Structure



Program Structure



The Challenge: A linear carbon economy for plastics



- Plastic is made from non-renewable feedstocks
- Plastic waste is increasingly accumulating¹
- Most of that plastic waste ends up in landfills and the environment²
- Plastic production currently consumes 6% of global oil and is anticipated to increase to 20% of global oil by 2050³

¹Geyer et al. Science Advances 2017

²Zheng and Suh. Nature Climate Change 2019

³Jambeck et al. Science 2015 and Ellen MacArthur Foundation

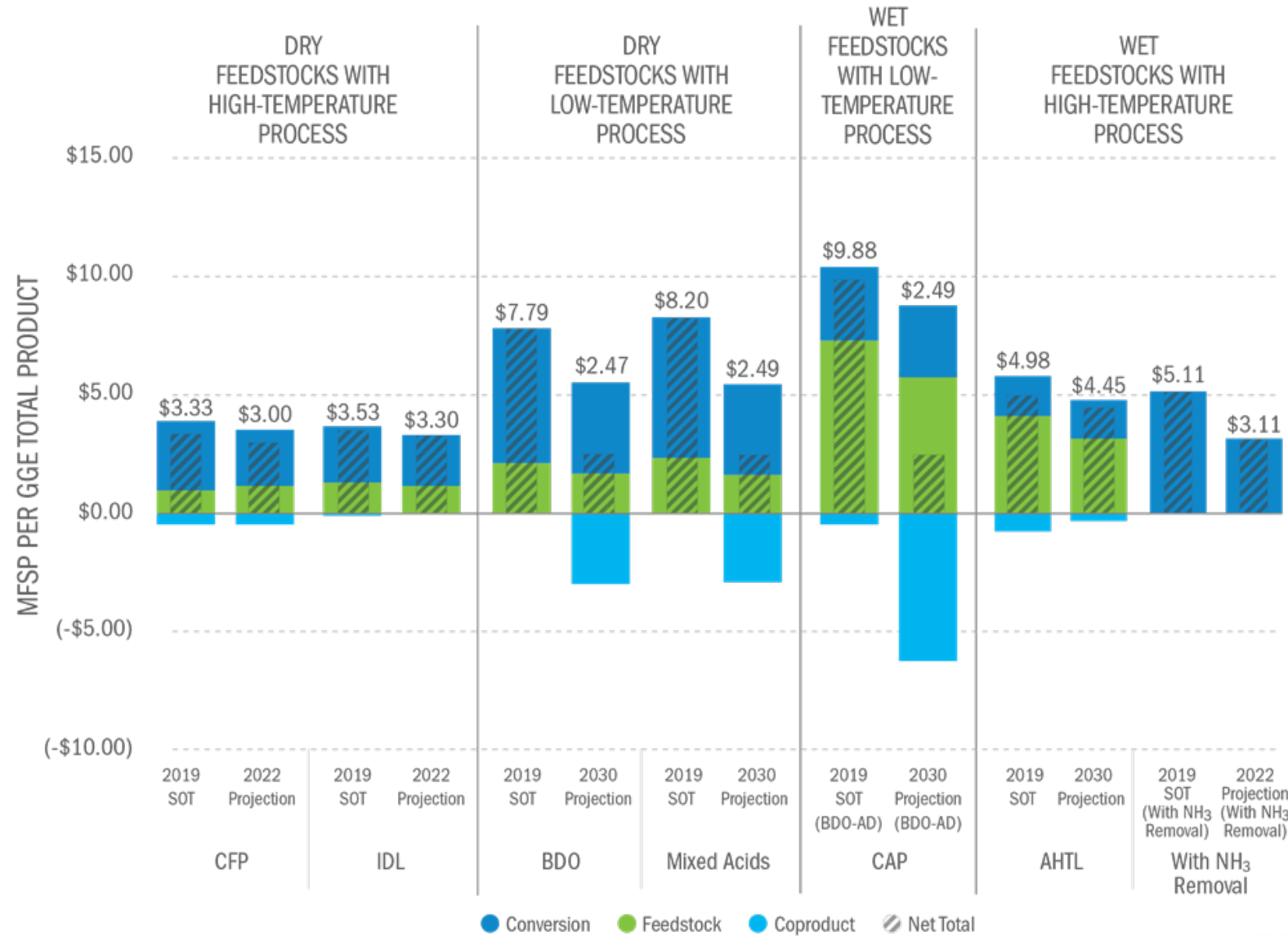
Challenges

- Pathway Specific Barriers
 - Deconstruction and Fractionation
 - Feedstock quality metrics
 - Efficient Preprocessing and Pretreatment
 - Synthesis and Upgrading Barriers
 - Process development for lignin conversion
 - Advanced bioprocess development
 - Increasing catalytic process yield
 - Decreasing catalyst development time
 - Waste Conversion Barriers
 - Gas fermentation
 - High moisture feedstock conversion beyond AD
 - Bioproducts Barriers
 - Identification and evaluation of potential co-products
 - Bio-based production synthesis

Challenges

- Enabling Research Barriers
 - Organism development
 - Reactor materials and analytical methods
 - Multi-scale computational framework for accelerating technology development
 - Separations
 - Selective separation of organic species
 - Selective separation of inorganic contaminants

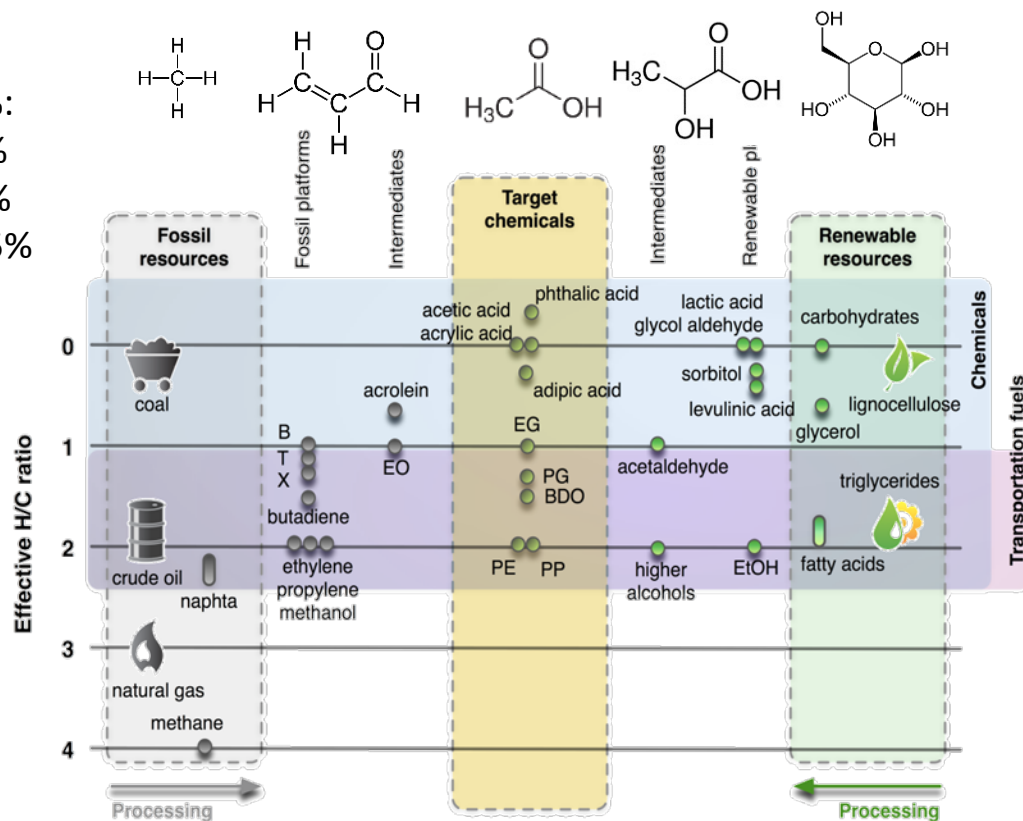
Technoeconomic Assessments (TEA) for Several Example Pathways



Biobased products contain oxygen... like biomass

Crude oil
 Avg. wt%:
 C 83-87%
 H 10-14%
 O 0.1-1.5%

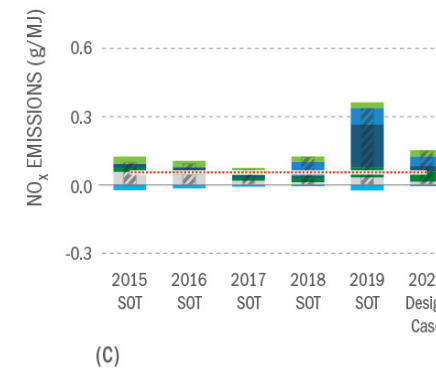
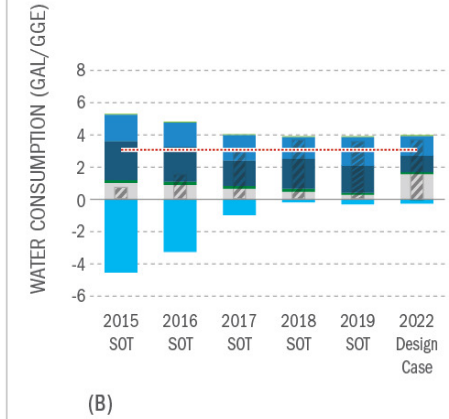
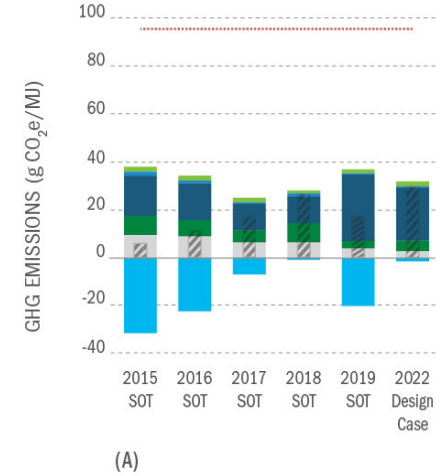
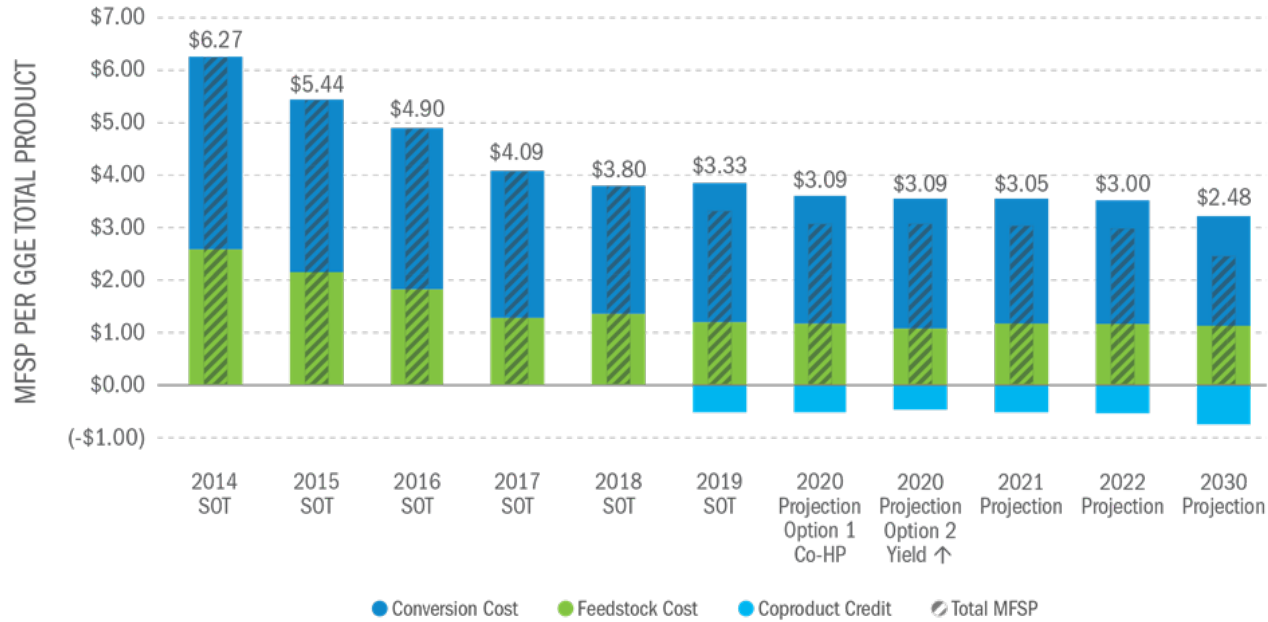
Biomass
 Avg. wt%:
 C 36-53%,
 H 5-7%,
 O 31-48%



Consider the oxidation state of chemicals – retain what nature provides

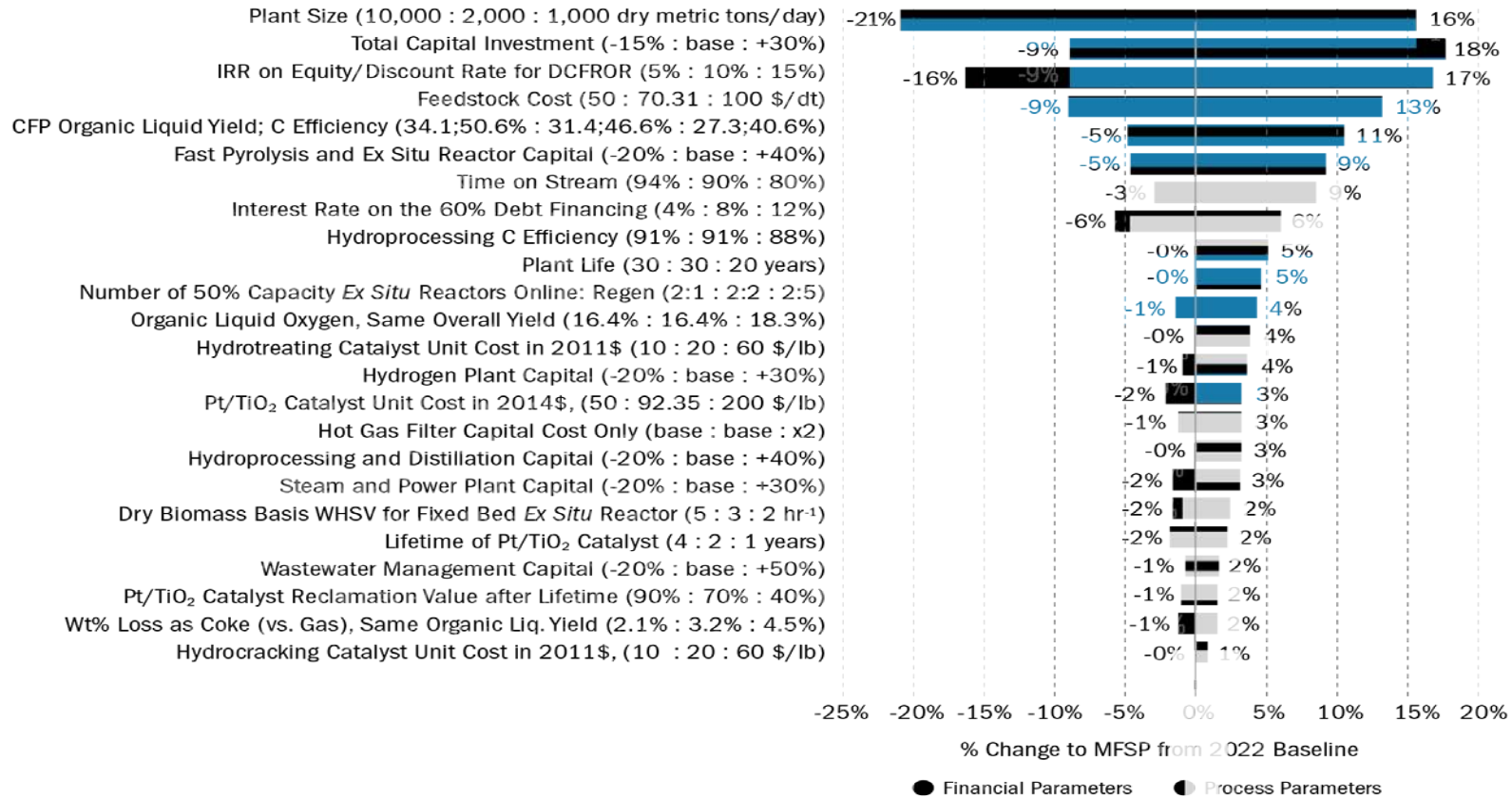
Vennestrøm, P.N. R. *et al Angew. Chem. Int. Ed.* **2011**, *50*, 10502-10509
 Shen, J. *et al Energy Conversion and Management* **2010**, *51*, 983-987

Catalytic Fast Pyrolysis – TEA and Sustainability Analysis



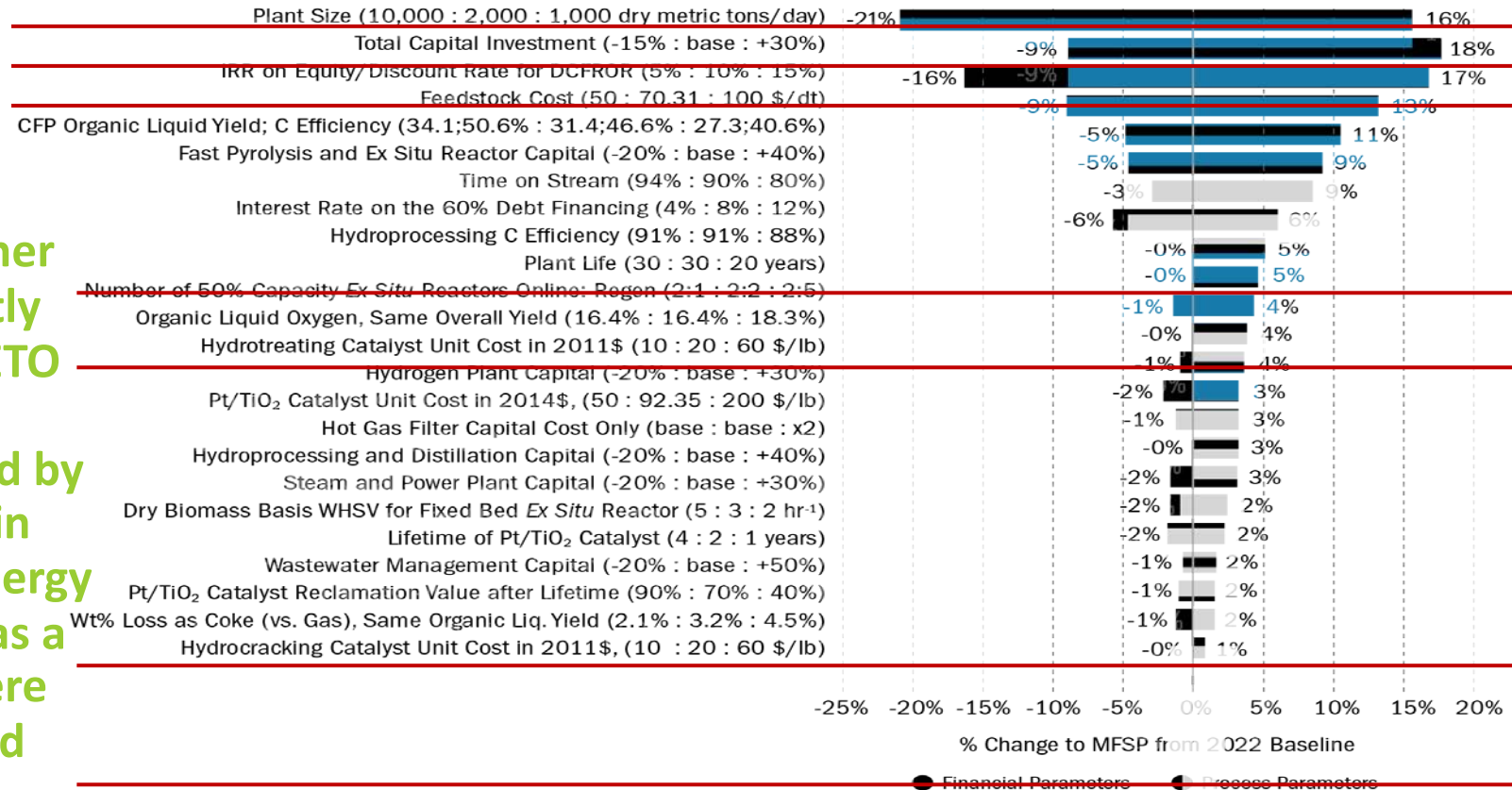
- Fuel Transportation and Net Fuel Combustion
- Biorefinery Conversion
- Depot Preprocessing
- Fieldside Preprocessing and Transportation to Depot
- Silviculture, Fertilization, Harvest, and Collection
- Supply Chain
- Coproduct Displacement Credits
- Petroleum gasoline

Ex-situ CFP



Ex-situ CFP

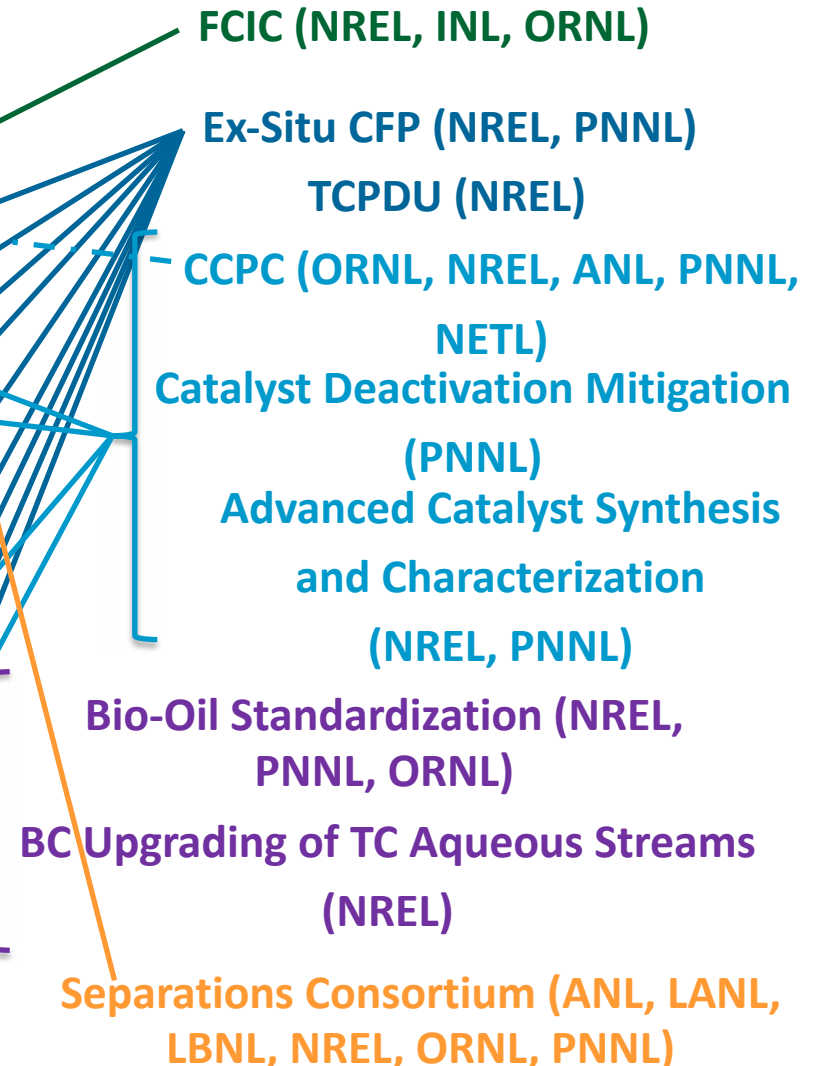
Items either not directly tied to BETO R&D or influenced by progress in the bioenergy industry as a whole were eliminated



Ex-situ CFP

Top 10 remaining areas by current active project:

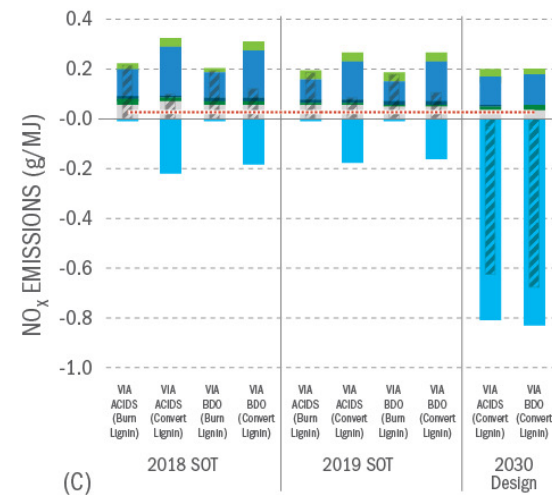
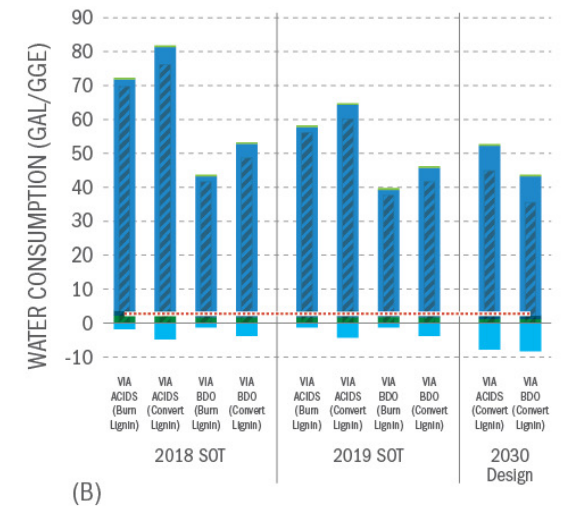
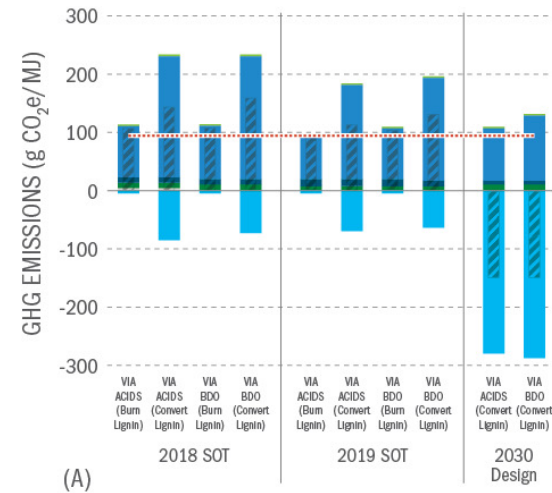
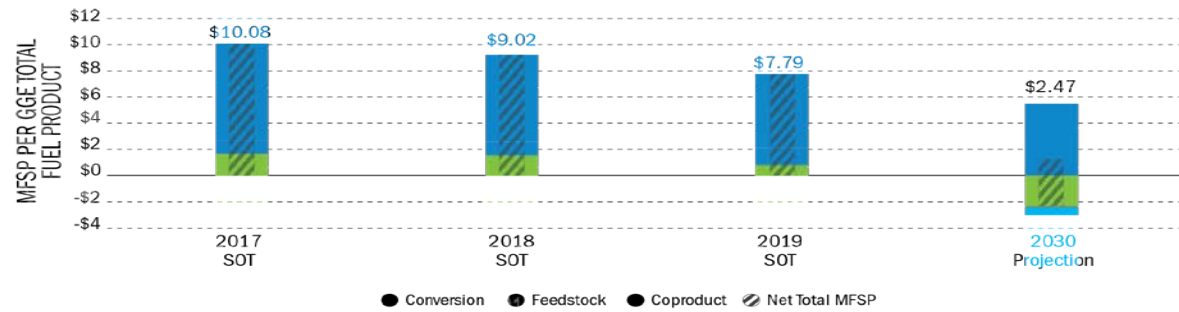
Rank	Description
1	Feedstock Cost, \$/dry U.S. ton
2	CFP Organic Liq. Yield; Carbon Efficiency %
3	Fast Py. & Ex Situ Reactor Capital
4	Time on Stream
5	Hydroprocessing C Efficiency %
6	No. of 50% Capacity Ex Situ Reactors Online:Regen
7	Organic Liq. Oxygen %, Same Overall Yield
8	Hydrotreating Catalyst Unit Cost
9	Hydrogen Plant Capital
10	Pt/TiO ₂ Catalyst Unit Cost



Investments in High Impact Barriers - Ex-situ CFP

Rank	Description	FY19	FY20	FY21
1	Feedstock Cost, \$/dry U.S. ton	\$1,500,000	\$2,000,000	\$2,000,000
2	CFP Organic Liq. Yield; Carbon Efficiency %	\$12,330,000	\$10,000,000	\$8,300,000
3	Fast Py. & Ex Situ Reactor Capital	\$4,450,000	\$3,400,000	\$1,700,000
4	Time on Stream	\$9,530,000	\$7,200,000	\$5,500,000
5	Hydroprocessing C Efficiency %	\$9,530,000	\$7,200,000	\$5,500,000
6	No. of 50% Capacity Ex Situ Reactors Online:Regen	\$4,450,000	\$3,400,000	\$1,700,000
7	Organic Liq. Oxygen %, Same Overall Yield	\$5,650,000	\$4,600,000	\$2,900,000
8	Hydrotreating Catalyst Unit Cost	\$9,530,000	\$7,200,000	\$5,500,000
9	Hydrogen Plant Capital	\$4,450,000	\$3,400,000	\$1,700,000
10	Pt/TiO2 Catalyst Unit Cost	\$9,530,000	\$7,200,000	\$5,500,000

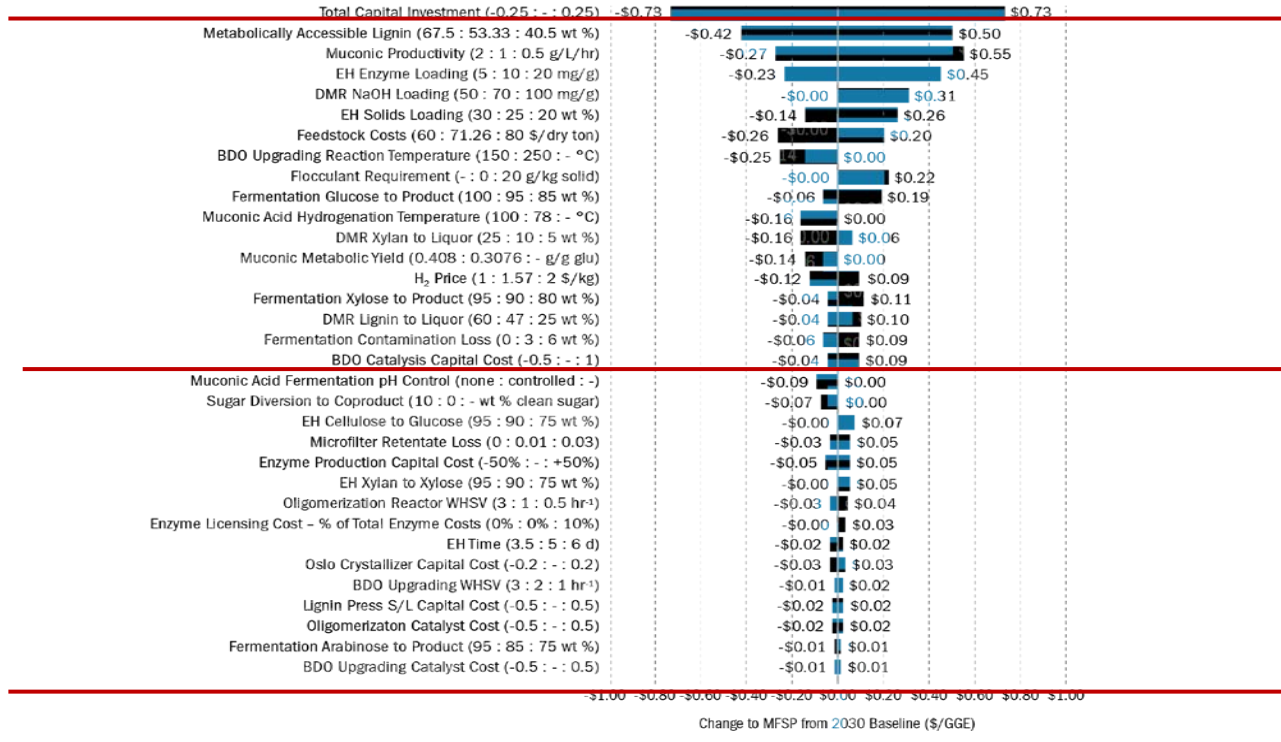
Biochemical Pathways – TEA and Sustainability Analysis



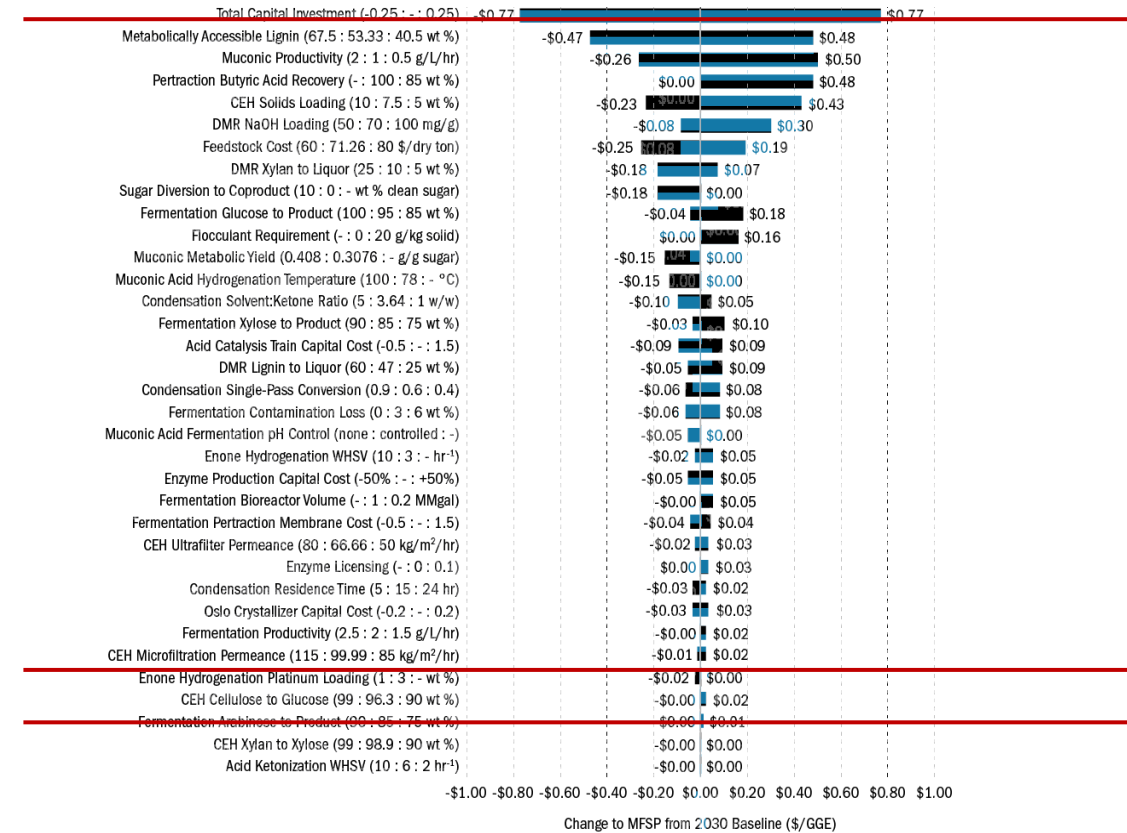
- Fuel Transportation and Net Fuel Combustion
- Biorefinery Conversion
- Depot Preprocessing
- Fieldside Preprocessing and Transportation to Depot
- Harvest and Collection
- Coproduct Displacement Credits
- ▨ Total Supply Chain
- Petroleum Diesel

Fuel price sensitivity – Biochemical Conversion Pathways

Biochemical – BDO



Biochemical – Acids



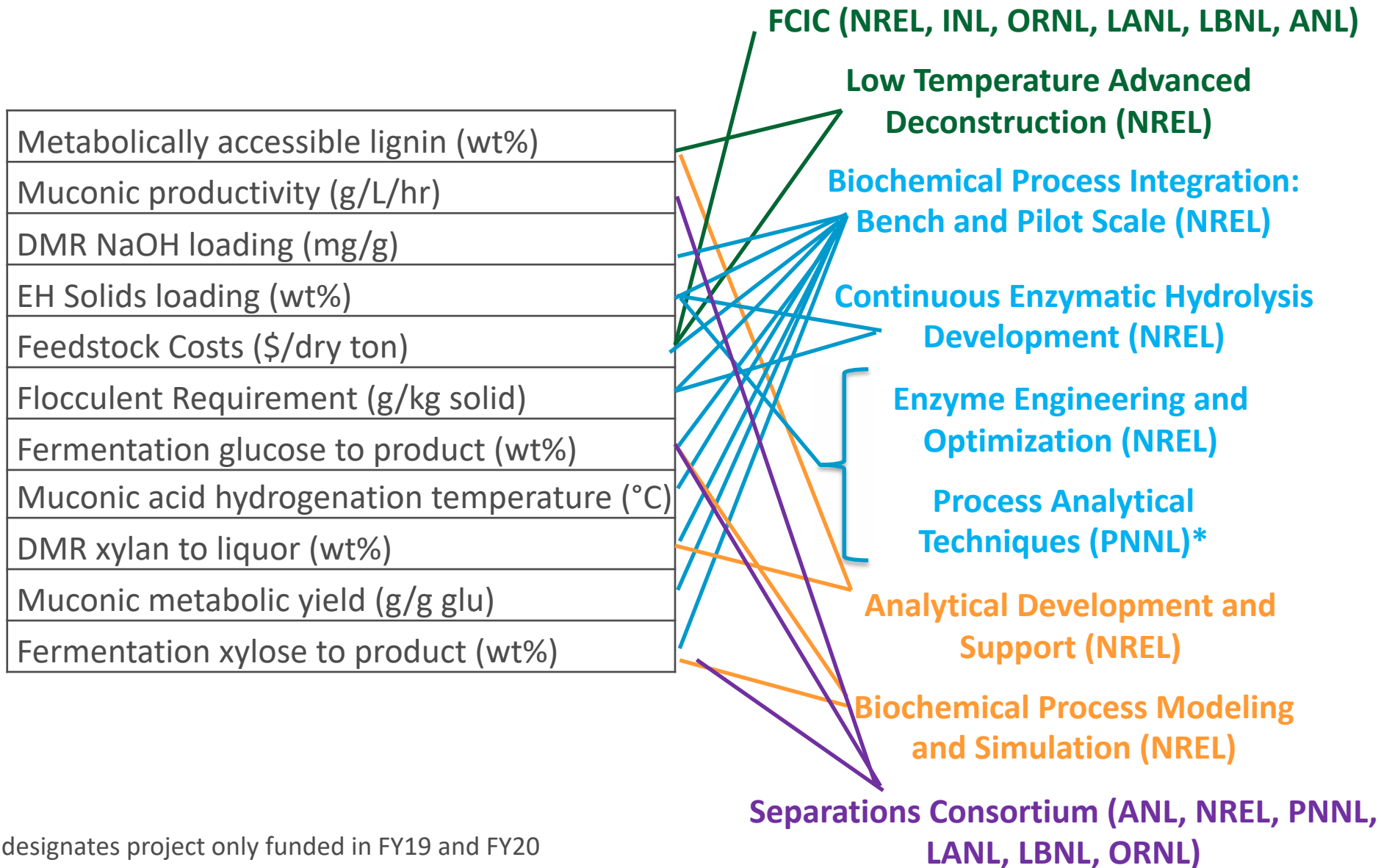
Biochemical – BDO/Acids (Lignin)

1	Metabolically accessible lignin (wt%)
2	Muconic productivity (g/L/hr)
3	EH enzyme loading mg/g
4	DMR NaOH loading (mg/g)
5	EH Solids loading (wt%)
6	BDO upgrading reaction temperature (°C)
7	Fermentation glucose to product (wt%)
8	Muconic acid hydrogenation temperature (°C)
9	DMR xylan to liquor (wt%)
10	Muconic metabolic yield (g/g glu)
11	Fermentation xylose to product (wt%)

- Low Temperature Advanced Deconstruction (NREL)**
- Oxidative Valorization of Lignin* (PNNL)**
- Electrocatalytic Oxidation of Lignin Oligomers* (NREL)**
- Gas Phase Selective Partial Oxidation of Lignin* (NREL)**
- Biological Lignin Valorization (NREL, SNL*)**
- Lignin Utilization (NREL)**
- Lignin First Biorefinery Development (NREL)**
- Synthetic Metabolic Pathways for Bioconversion of Lignin (ORNL)**
- Multiple competitive selections made in FY19 and FY20**

*designates project only funded in FY19 and FY20

Biochemical – BDO/Acids (other overlapping areas)



*designates project only funded in FY19 and FY20

Investments in High Impact Barriers – Biochemical Pathways

Biochemical – BDO

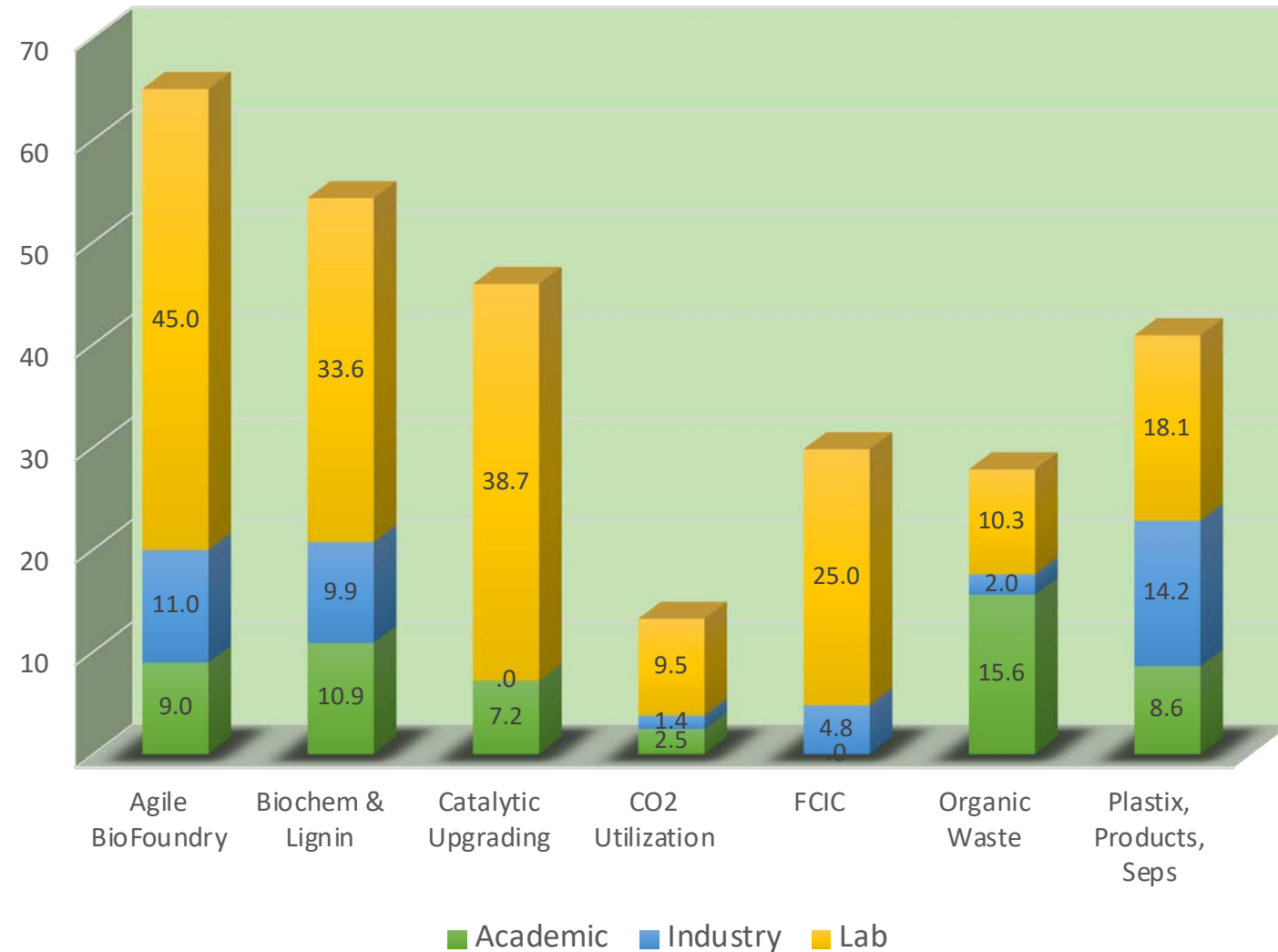
	Description	FY19	FY20	FY21
1	Metabolically accessible lignin (wt%)	\$6,500,000	\$6,220,000	\$5,370,000
2	Muconic productivity (g/L/hr)	\$5,650,000	\$5,650,000	\$5,650,000
3	EH enzyme loading mg/g	\$3,950,000	\$3,950,000	\$3,700,000
4	DMR NaOH loading (mg/g)	\$2,250,000	\$2,250,000	\$2,250,000
5	EH Solids loading (wt%)	\$3,400,000	\$3,400,000	\$3,150,000
6	Feedstock Costs (\$/dry ton)	\$1,500,000	\$2,000,000	\$2,000,000
7	Flocculant Requirement (g/kg solid)	\$1,300,000	\$1,300,000	\$1,300,000
8	BDO upgrading reaction temperature (°C)	\$4,050,000	\$4,050,000	\$4,050,000
9	Fermentation glucose to product (wt%)	\$8,500,000	\$8,500,000	\$8,500,000
10	Muconic acid hydrogenation temperature (°C)	\$2,250,000	\$2,250,000	\$2,250,000
11	DMR xylan to liquor (wt%)	\$5,700,000	\$5,570,000	\$5,570,000
12	Muconic metabolic yield (g/g glu)	\$2,250,000	\$2,250,000	\$2,250,000
13	Fermentation xylose to product (wt%)	\$8,500,000	\$8,500,000	\$8,500,000

Biochemical – Acids

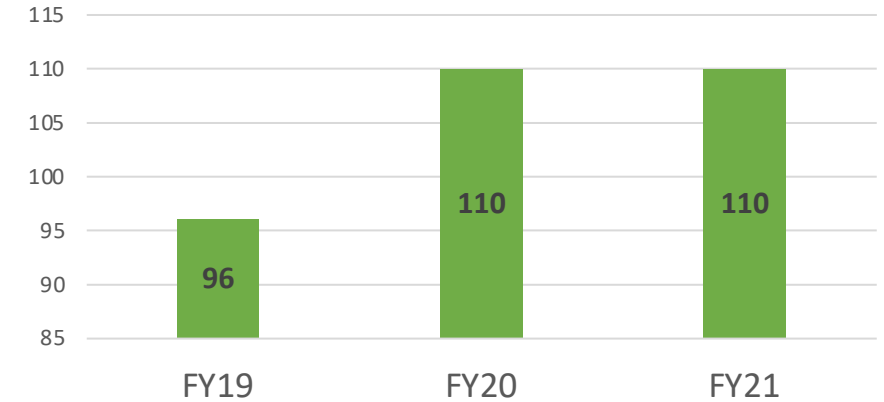
	Description	FY19	FY20	FY21
1	Metabolically accessible lignin (wt%)	\$6,500,000	\$6,220,000	\$5,370,000
2	Muconic productivity (g/L/hr)	\$5,650,000	\$5,650,000	\$5,650,000
3	Pertraction butyric acid recovery (wt%)	\$4,150,000	\$4,150,000	\$4,150,000
4	CEH Solids loading (wt%)	\$3,950,000	\$3,950,000	\$3,700,000
5	DMR NaOH loading (mg/g)	\$2,500,000	\$2,500,000	\$2,250,000
6	Feedstock Cost (\$/dry ton)	\$1,500,000	\$2,000,000	\$2,000,000
7	Flocculant Requirement (g/kg solid)	\$1,300,000	\$1,300,000	\$1,300,000
8	DMR xylan to liquor (wt%)	\$3,050,000	\$2,920,000	\$2,920,000
9	Sugar diversion to coproduct (wt% clean sugar)	\$750,000	\$750,000	\$750,000
10	Fermentation glucose to product (wt%)	\$8,050,000	\$8,050,000	\$7,650,000
11	Muconic metabolic yield (g/g sugar)	\$4,900,000	\$4,900,000	\$4,900,000
12	Muconic acid hydrogenation Temperature (°C)	\$2,250,000	\$2,250,000	\$2,250,000
13	Condensation solvent:ketone ratio (w/w)	\$2,100,000	\$2,100,000	\$1,700,000
14	Fermentation xylose to product (wt%)	\$5,800,000	\$5,800,000	\$5,400,000

Budget totals for years under review

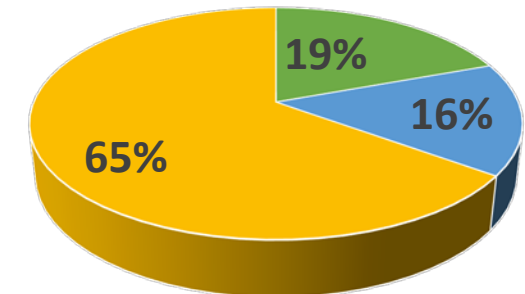
Reviewed Project Budgets (\$M)



Annual Conversion R&D Budget (\$M)



Funding Distribution



■ Academic ■ Industry ■ Lab

Recent Conversion R&D Funding Opportunity Announcements

FY19 FOA Topics	Available Funding
Renewable Energy from Urban and Suburban Wastes	\$10,000,000
Advanced Bioprocessing	\$5,000,000
Agile Biofoundry	\$5,000,000
Designing Highly Recyclable Plastics	\$5,000,000
Designing Novel Methods for Deconstructing and Upcycling Existing Plastics	\$5,000,000
Rethinking Anaerobic Digestion	\$5,000,000
Biopower and RNG	\$5,000,000

FY20 FOA Topics	Available Funding
Waste to Energy Strategies for the Bioeconomy: 2a: Municipal Solid Waste (MSW) 2b: Optimizing Community Scale Wet Organic Wastes	\$2,500,000
Biopower and Products from Urban and Suburban Wastes: North American Multi-University Partnership for Research and Education: 6a: Biopower from Organic Wastes 6b: Waste Plastics to Products	\$15,000,000
Scalable CO ₂ Electrocatalysis	\$8,000,000

Recent Conversion R&D SBIR topics and Directed Funding Opportunities

SBIR Topics	Available Funding
Cell-Free Biochemical Platforms to Optimize Biomass Carbon Conversion Efficiency (FY19 Phase 1, Release 2)	\$806,497
Cell-Free Biochemical Platforms to Optimize Biomass Carbon Conversion Efficiency (FY20 Phase 2, Release 2)	\$1,098,268
BOTTLE/PIC	\$4,500,000

Directed Funding Opportunities	Available Funding
Agile BioFoundry Directed Funding Opportunity (FY20)	\$5,700,000
Consortium for Computational Physics & Chemistry	\$1,032,000
ChemCatBio (CCB)	\$980,000

Key Accomplishments

Technology Area	Key Technical Advance(s)
Biochemical Conversion and Lignin Utilization	<p>Biochemical Conversion:</p> <ul style="list-style-type: none"> Developed and published major organism engineering strategies used to optimize the organism at the center of the anaerobic fermentation of sugars to carboxylic acids pathway. This new strain can produce over 85 g/L butyric acid and still maintain cell growth at that high product concentration. Cell-Free Biosynthesis: Demonstrated Glucose <i>and</i> Xylose co-utilization in Cell-free Biosynthesis with near 60% yield on hydrolysate <p>Lignin:</p> <ul style="list-style-type: none"> Developed and industrially-relevant process concept for lignin-first processing for the first time Conducted first comprehensive TEA and LCA for reductive catalytic fractionation of lignin Demonstrated stable lignin oil production for the first time Developing continuous RCF with high BP solvents Improvements in lignin analytics (via the LigninWrangler computational tool) to generate lignin structure libraries as well as lignin-derived molecules resulting from deconstruction chemistries Biological approaches: Developed <i>P. putida</i> strains and bioprocesses able to achieve near industrially-relevant TRY (~49g/L muconate); Discovered novel biological underpinnings of lignin degradation
CCB & CCPC	<ul style="list-style-type: none"> Licensing of ORNL's ethanol-to-butadiene-jet (ETBJ) technology to Prometheus Fuel Sironix Renewables DFA and LANL received the R&D 100 Special Recognition: Green Tech R&D World magazine awarded a bronze special recognition to Sironix and LANL for their work on oleo-furan surfactants made from renewable biomass. ChemCatBio Consortia continues to improve research efficiency and accelerate catalyst-process development cycle through publicly available tools: The CatCost™ Tool continues to expand, showing high utilization rates by researchers: in 2020 the tool had 1,492 users / 2,077 sessions. https://catcost.chemcatbio.org/. In 2020, the ChemCatBio Data Hub project developed and publicly released the Catalyst Property Database https://cpd.chemcatbio.org/: curation and standardization of 3000+ datasets currently.

Key Accomplishments

Technology Area	Key Technical Advance(s)
ABF	<p>Publications: 250+ citations across 50 publications to date (since FY17 – many are since FY19) 67 citations across 17 publications since FY20</p> <p>Patents:</p> <ul style="list-style-type: none"> • 16 patent applications; 6 records of invention; 7 software disclosures; 5 licenses • 18 partnerships with industry & academia (let me know if you want the NASCAR slide below) • Developed Beachhead concept and metabolic map • Exceeded FY20 annual milestone: “Demonstrate at least one representative target of a beachhead at a TRY of 20 g/L, 0.3 g/L/hr, and 50% of theoretical yield” Acontic acid was produced using <i>Aspergillus pseudoterreus</i>, exceeding the titer goal of 20 g/L by 130%, exceeding the rate goal of 0.3 g/Lh by 27%, and coming within 96% of the yield goal.
Separations	<ul style="list-style-type: none"> • Separations applications: product separation and recovery, impurity/foulant removal, new material development. • Separation technologies developed: adsorption, extraction-distillation, membranes, catalytic hot gas filtration, capacitive deionization, electrodeionization, and countercurrent chromatography. • 9 journal publications, 3 patent applications since 2019. • Three year overview published, outlining the progress made over the first three years
CO2 Utilization	<ul style="list-style-type: none"> • NZTT: Performed TEA and LCA on several renewable fuel pathways to understand the potential and the cost for "efuels" to achieve net-zero carbon intensity. • Completed a three-year study into the overall feasibility of CO2 reduction and to produce technical information to inform an aggressive R&D strategy in the field • Issued and awarded 3 FOA awards to develop scalable CO2 electrolyzers (Dioxide Materials, University of Delaware, Opus 12)

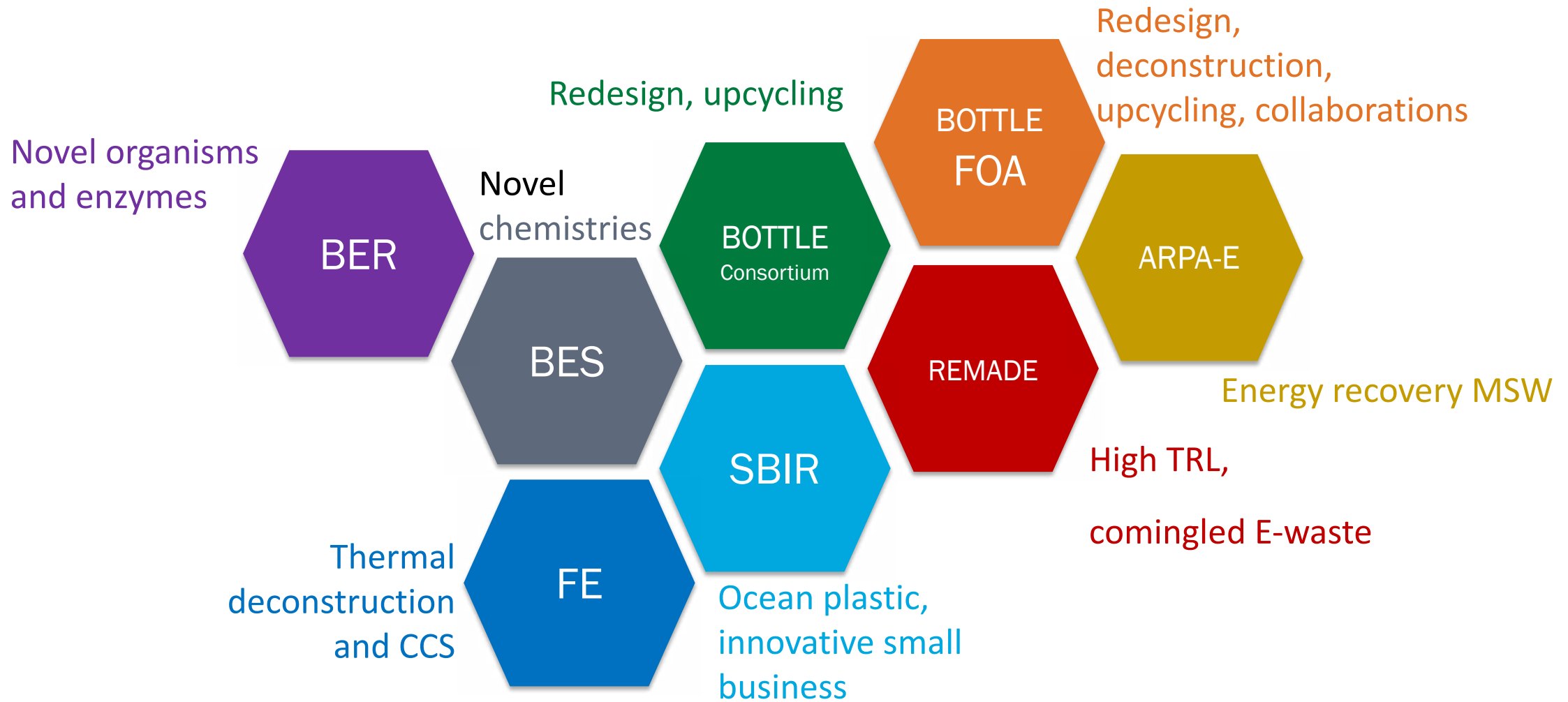
Key Accomplishments

Technology Area	Key Technical Advance(s)
Waste Utilization	<ul style="list-style-type: none"> • Site-specific organic waste availability survey • Engine testing of HTL fuels • Process for conversion of volatile fatty acids (e.g. from AD) to sustainable aviation fuels • RNG from biogas - SoCalGas/Electrochaeta project • Improved Anaerobic Digestion technologies and reactor design
Performance advantaged bioproducts	<ul style="list-style-type: none"> • 100 new polymer formulations and identified 11 new products that can be classified as performance-advantaged relative to a petroleum standard in at least one material property. <ul style="list-style-type: none"> T_g Flame resistance Biodegradability. • Development of a computational tool for identifying novel polymers <ul style="list-style-type: none"> Released to the public later this year Forthcoming <i>Nature</i> article in late spring 2021 that proposes a standard framework for how to identify and design PABPs.
Plastics	<ul style="list-style-type: none"> • BOTTLE Consortium kicked off and FOA issued both in partnership with the Advanced Manufacturing Office • Request for information issued for Plastics Innovation Challenge roadmap

Future Directions

- SAF Emphasis
- BOTTLE
- CO2 conversion
- Waste to fuels

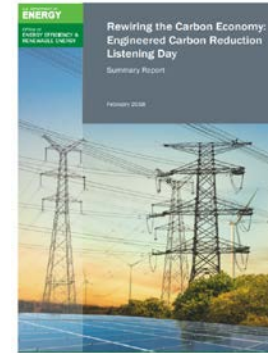
What can DOE do?



DOE's Plastics Innovation Challenge

Background on CO₂-to-Fuels in BETO

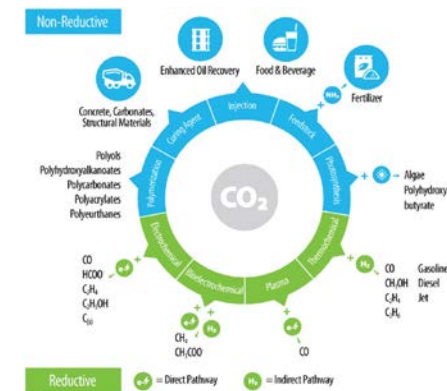
- **FY17: BETO began investigating CO₂ utilization**
 - Hosted a workshop in July 2017
 - Leveraged SBIR program to understand the current state of technology
 - Initiated a *Feasibility Study* at NREL to get a firm view on technical barriers
- Informed a strategy that took advantage of BETO's existing portfolio structure
- **FY18 FOA:** sought entities that could perform CO₂ reduction to team with those w/expertise in upgrading
- **FY20 FOA: Scalable CO₂ Electrocatalysis**, hosted a CO₂ Summit and issued a questionnaire to the labs
- Now understand the challenges and barriers, and we wish to address them with a larger targeted effort at the National Labs



Transforming the carbon economy: challenges and opportunities in the convergence of low-cost electricity and reductive CO₂ utilization?

R. Gary Grim, Zhe Huang, Michael T. Guarnieri, Jack R. Ferrell III, Ling Tao and Joshua A. Schaidle

The increasing availability of renewable electricity at costs competitive with, and even lower than, electricity from fossil sources along with growing interest and recent technological advancements in reducing carbon emissions through CO₂ capture is challenging the status quo in the way that we produce and consume energy and products. Renewable electricity can be leveraged to produce fuels and chemicals from CO₂, offering sustainable routes to reduce the carbon intensity of our energy and products-driven economy. A number of approaches have been developed for the electron-driven reduction of CO₂ to products, including both direct and indirect (via an energy carrier such as H₂) pathways and spanning from electrochemical to biological to thermocatalytic conversion. While these approaches are at various stages of development, there are technical barriers related to each core conversion technology that need to be addressed in order to accelerate commercialization and drive the transition towards a circular carbon economy. In this perspective, we assess and characterize the top technical barriers for utilizing renewable electricity for CO₂ reduction across five different conversion approaches (direct electrochemical, direct bioelectrochemical, direct non-thermal plasma, indirect bioelectrochemical, and indirect thermochemical) under state-of-technology conditions, outline the R&D needs to overcome each barrier, and identify the most promising C₁-C₄ hydrocarbons and oxygenates based on their relative ease of formation, economic viability, CO₂ utilization potential, and energy storage capacity. Our analysis suggests, based on current reported states of technology, that indirect pathways paired with the formation of C₁ products offer the most technically feasible approach for electron driven CO₂ reduction in the near term. However, as we strive for longer carbon chain molecules, and as technologies continue to advance, there are a multitude of advantages and limitations to be considered for all five approaches.



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THANK YOU REVIEWERS (and attendees)!



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