NREL
Transforming ENERGY

DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Biochemical Platform Analysis – 2.1.0.100

April 6, 2023
Biochemical Conversion & Lignin Valorization
Ryan Davis
NREL

Project Overview

Goal:

- Provide **process design and economic analysis support** for the biochemical conversion platform, to **guide R&D priorities based on economic + sustainability drivers**
  - Translate demonstrated/proposed research advances into product selling prices)

Outcomes:

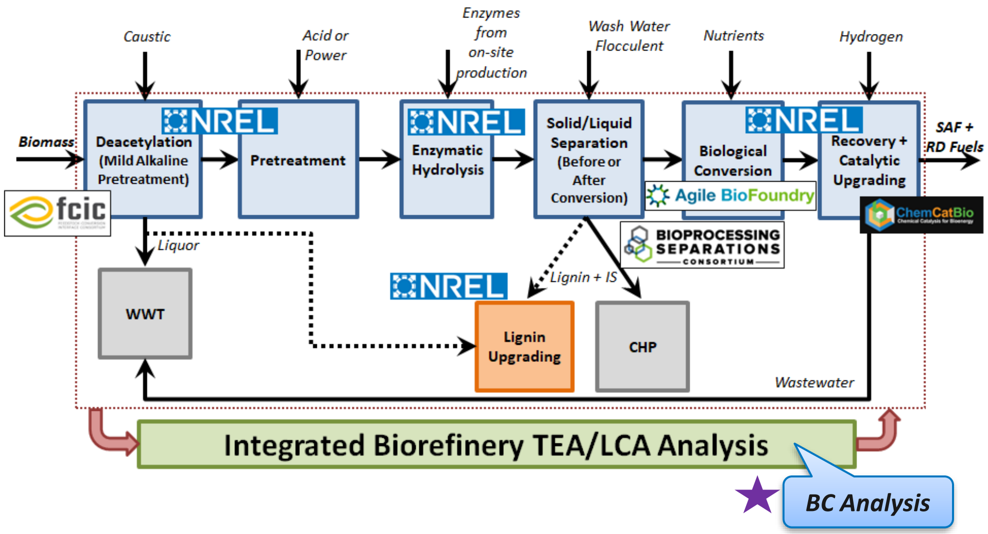
- Heilmeier Catechism:
  - Aim: Assess commercial potential for biochemical pathways via TEA modeling – **link R&D to biorefinery economics**
  - How done today: Linear approach: Aspen modeling → TEA → LCA (w/ ANL) – working to **co-optimize TEA+LCA jointly**
  - Importance: Work to **prioritize research** – identify impact of key variables and design alternatives on overall economics + carbon intensity
  - Risks: Ensure modeled designs are **commercially relevant**

Context:

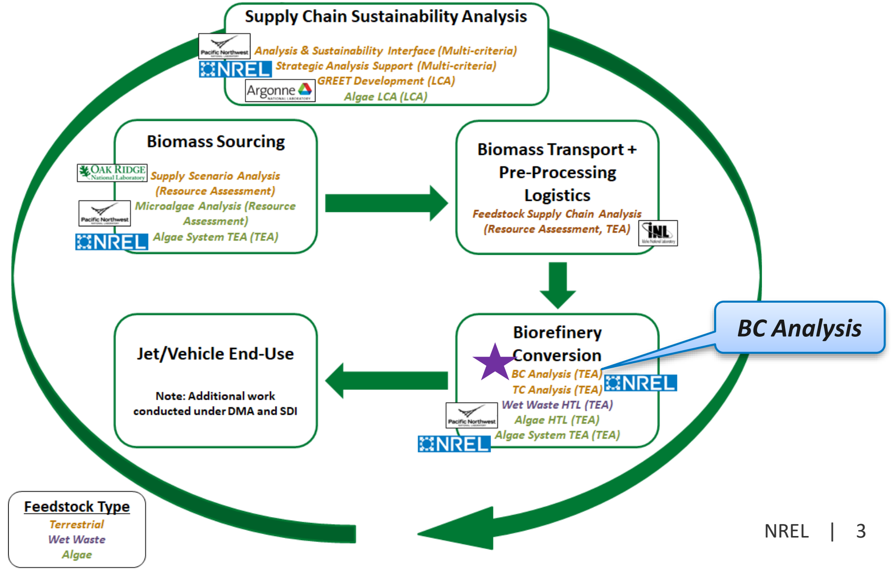
- This project **directly supports the BETO Program** by providing "bottom-up" modeling to show R&D needs for achieving "top-down" BETO goals (cost, GHG, etc)
- 20+ year history of **high-impact modeling** – widely-circulated reports since 1999 Wooley et al. ethanol report

1. Approach

- **Highly integrated with R&D efforts** – proactive assistance in R&D planning
- Substantial collaboration with NREL researchers, consortia partners spanning the value chain
- Also serve as a support task to evaluate TEA/LCA directly for others lacking dedicated budgets
  - Ex: TEA *directly leveraged to guide R&D directions* for CUBI, 2-stage deacetylation, BDO fermentation configurations, CEH vs batch EH



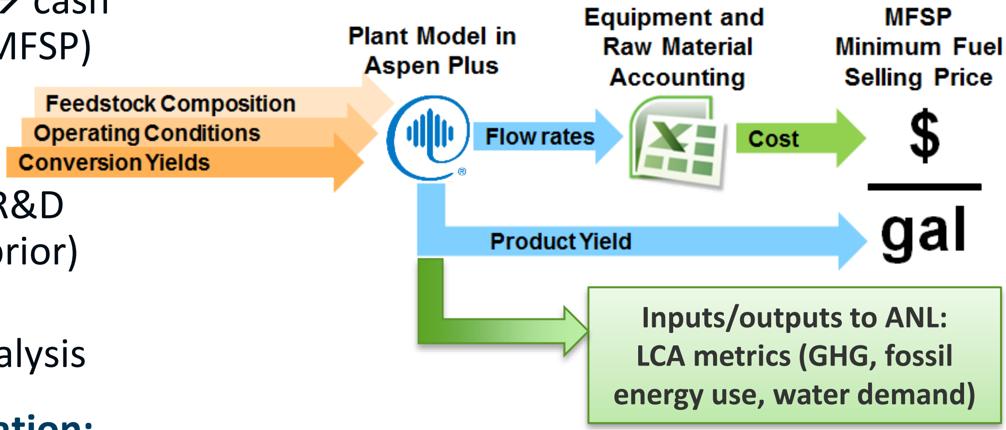
- **Strong collaboration with other analysis projects** – harmonize analysis for bigger picture
- Monthly calls to update other analysis projects, exchange information, plan milestones
- *Increased priorities moving forward on LCA* = frequent interactions with ANL, export Aspen model outputs for consistent TEA + LCA results



1. Approach

Technical Approach:

- Aspen Plus modeling for rigorous M&E balances → cash flow calculations set minimum fuel selling price (MFSP)
- Credibility of analysis supported by expert consultants, vetting with external stakeholders
- TEA has guided evolution of Platform directions, R&D focus since 2013 shift to hydrocarbon fuels (and prior)
- Measure progress through annual SOTs, prioritize future **R&D "bang for the buck"** via sensitivity analysis



Risks/Challenges:

- Risk: Single-dimensional analysis that optimizes for TEA at expense of LCA
- Risk: Premature down-selection to an infeasible pathway at expense of an alternate option
- Challenge: Specific MFSP targets require complex biorefinery configurations – commercial relevance?

Mitigation:

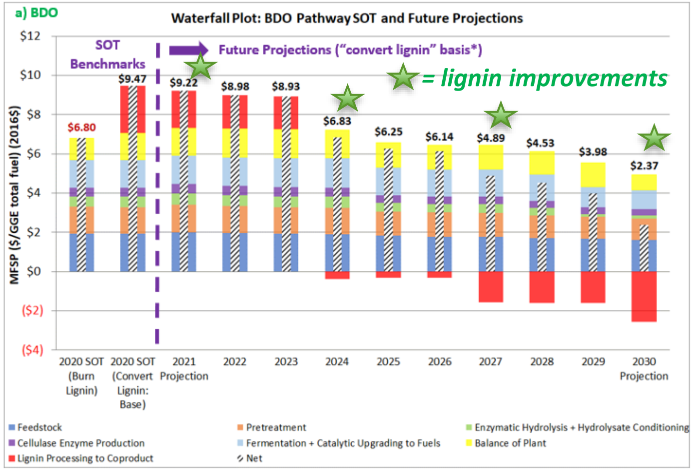
- Working closely with ANL partners for quicker LCA automation, co-optimization across multiple criteria
- Keep "all eggs out of one basket", continuously re-assess benchmark cases against new concepts
- BETO *moving away from specific MFSP targets*; future design cases will prioritize decarbonization, scale-up practicality + industry drivers

1. Approach

Management Approach:

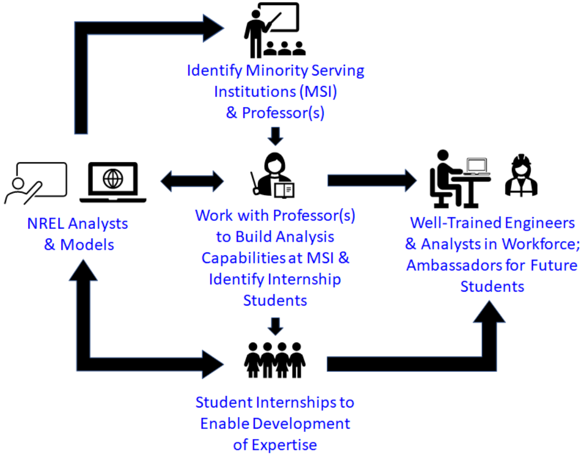
- Approach is guided by milestones:
  - TEA/LCA support for R&D projects
  - Refine/improve our tools and capabilities
  - Guidance for overall BC Platform
- Project structure: emphasis on process engineering expertise
  - Ryan Davis (PI) and 3+ process engineers support this project
  - Work with engineering subcontractors to improve model fidelity
- FY23 path forward: focus on **more engagement from industry**
  - **Go/No-Go** pathway down-select in FY23 (Q3) for future focus in FY24 design report update *(SAF + bio-products)*
  - Emphasis will be on *maximizing GHG reduction* while considering *commercial deployment potential* + industry-relevant technology

FY21 Go/No-Go – Establish Out-Year Goals for BC Platform (Guided by TEA)



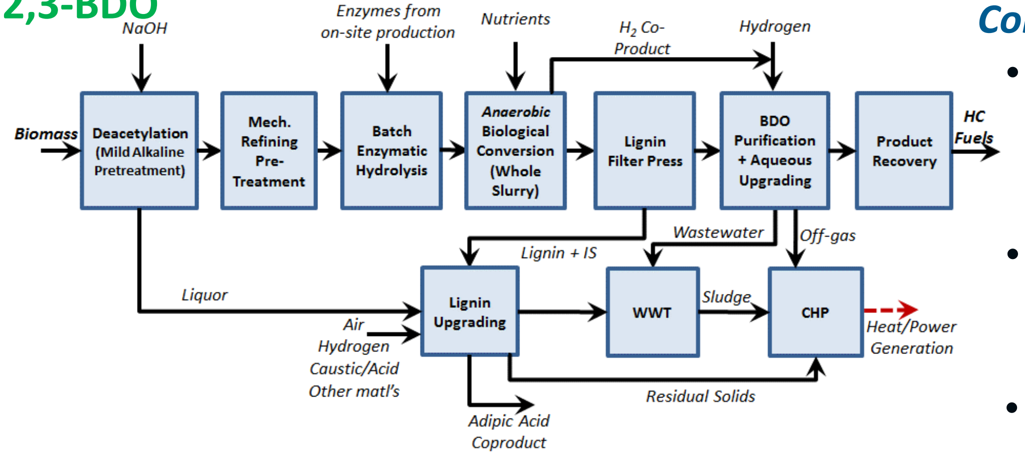
Diversity, Equity, and Inclusion:

- DEI goals established by pooling resources in TEA group (includes BC Analysis, TC Analysis, Algae TEA, Strategic Support)
- Goal: Establish working relationship with MSI university, help them develop TEA/LCA capabilities
  - FY25 DEI milestone: Joint manuscript with 1 or more MSI university collaborator (professor + student group) on TEA/LCA analysis

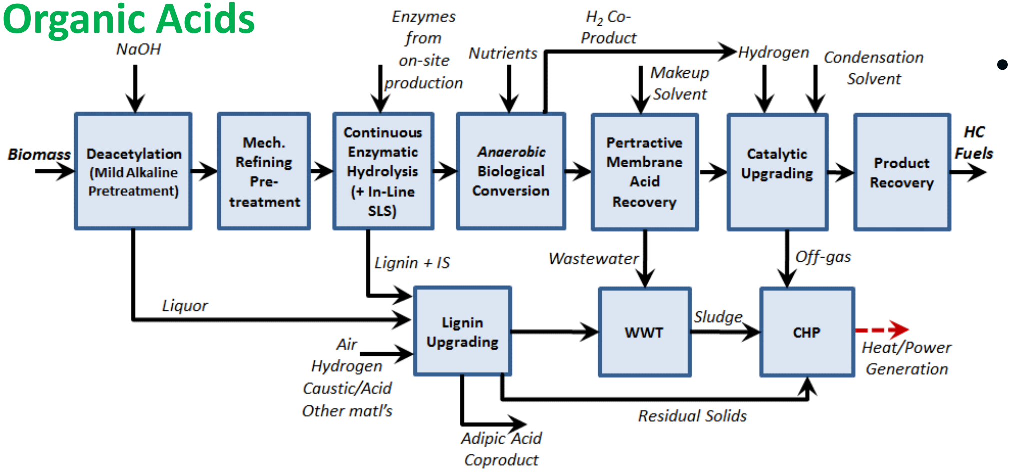


2. Progress and Outcomes

2,3-BDO

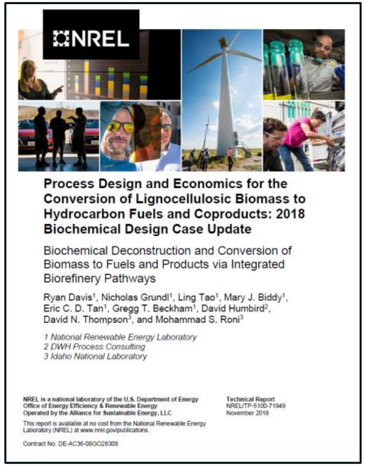


Organic Acids



Context: Pathways Investigated Under BC Platform

- Two pathways investigated, per 2018 NREL "design report":
  - 2,3-BDO to fuels
  - C4 acids to fuels
- Both pathways include lignin deconstruction + upgrading to coproducts (adipic acid as example)
- BDO: Batch EH + whole-slurry fermentation, aqueous upgrading
- Acids: Continuous EH (w/ solids removal), clarified sugar fermentation, pertractive acid recovery + upgrading


NREL

Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update

Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Pathways

Ryan Davis[1], Nicholas Grundl[1], Ling Tao[1], Mary J. Biddy[1], Eric C. D. Tan[1], Gregg T. Beckham[1], David Humbird[2], David N. Thompson[3], and Mohammad S. Roni[3]

1 National Renewable Energy Laboratory
2 DWH Process Consulting
3 Idaho National Laboratory

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Contract No. DE-AC36-08GO28308

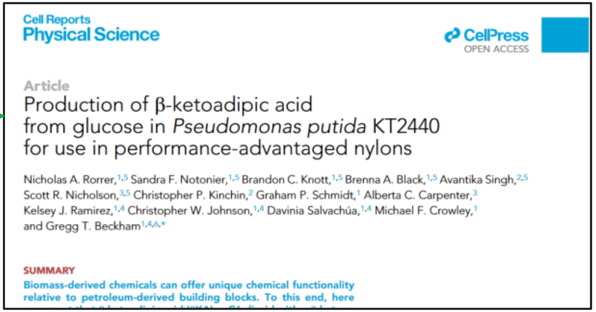
Technical Report NREL/TP-5100-71949 November 2018

https://www.nrel.gov/docs/fy19osti/71949.pdf

2. Progress and Outcomes

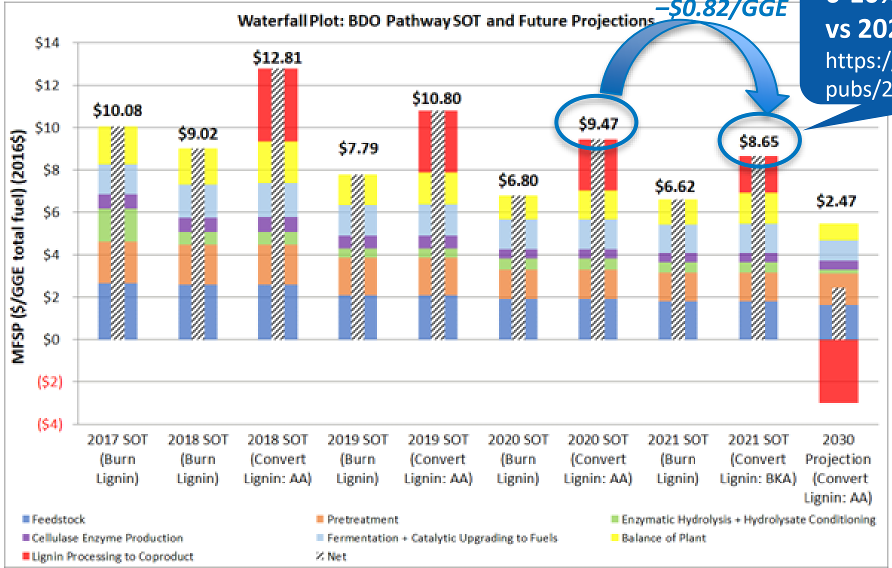
2021 SOT Demonstrates Improvements to Lignin Coproduct Valorization

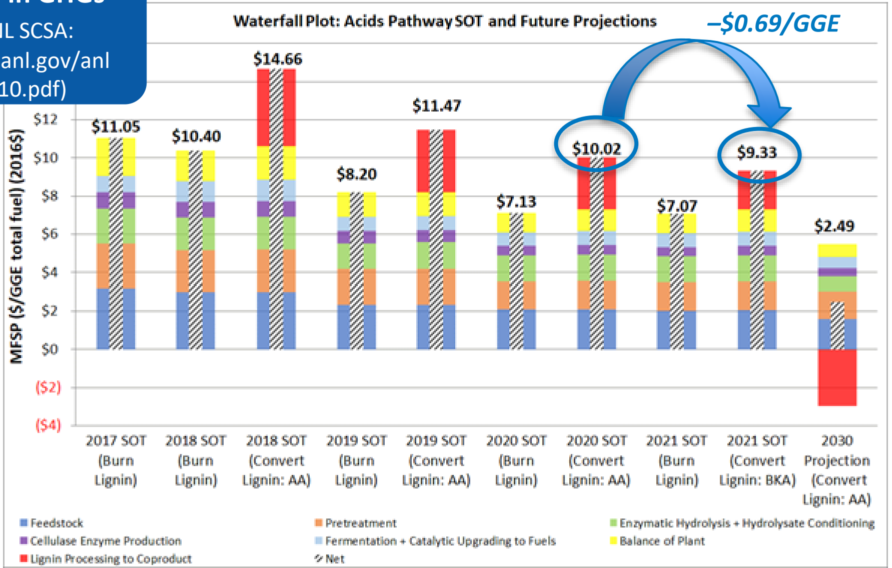
- 2021 SOT focused on lignin conversion to coproducts
- Replaced AA with BKA coproduct via lignin monomer bioconversion
- Synergies with other BETO work: BKA imparts superior thermal properties to resultant end-product (nylon-6,6)
- 19% improvement in yield + 4X increase in productivity (key cost driver) = key contributor to **$0.69-$0.82/GGE MFSP reduction** versus 2020 SOT lignin-to-AA


Cell Reports Physical Science
CelPress OPEN ACCESS
Article
Production of β-ketoadipic acid from glucose in *Pseudomonas putida* KT2440 for use in performance-advantaged nylons
Nicholas A. Rorrer,[1,5] Sandra F. Notonier,[1,5] Brandon C. Knott,[1,5] Brenna A. Black,[1,5] Avantika Singh,[2,5] Scott R. Nicholson,[3,5] Christopher P. Kinchin,[2] Graham P. Schmidt,[1] Alberta C. Carpenter,[3] Kelsey J. Ramirez,[1,4] Christopher W. Johnson,[1,4] Davinia Salvachúa,[1,4] Michael F. Crowley,[1] and Gregg T. Beckham[1,4,6,*]
SUMMARY
Biomass-derived chemicals can offer unique chemical functionality relative to petroleum-derived building blocks. To this end, here

Cell Reports Physical Science 3 (2022), 100840

6-10% reduction in GHGs vs 2020 SOTs (ANL SCSA: https://publications.anl.gov/anlpubs/2022/04/174410.pdf)

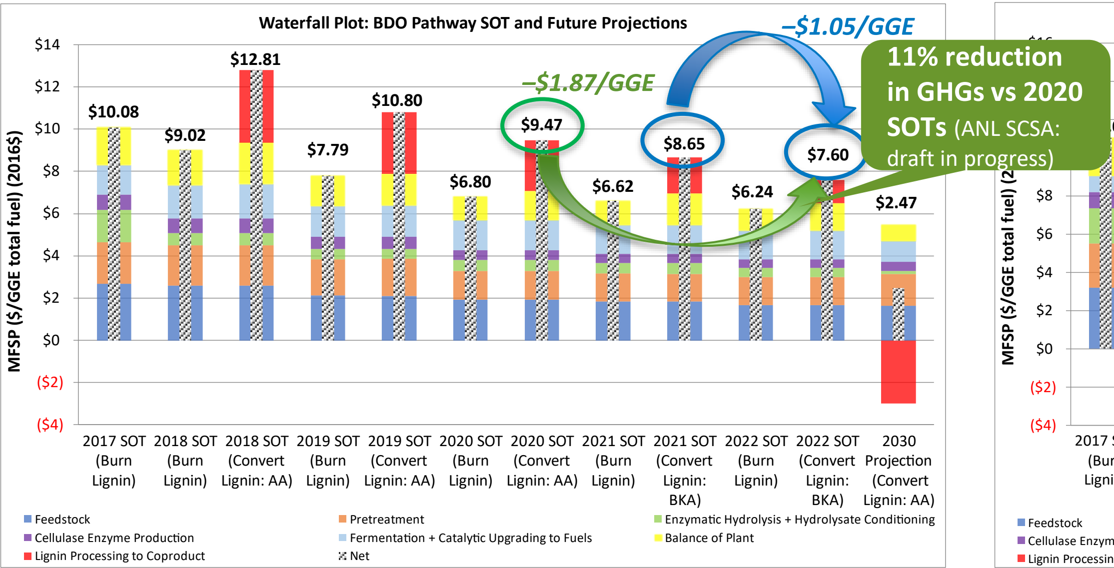


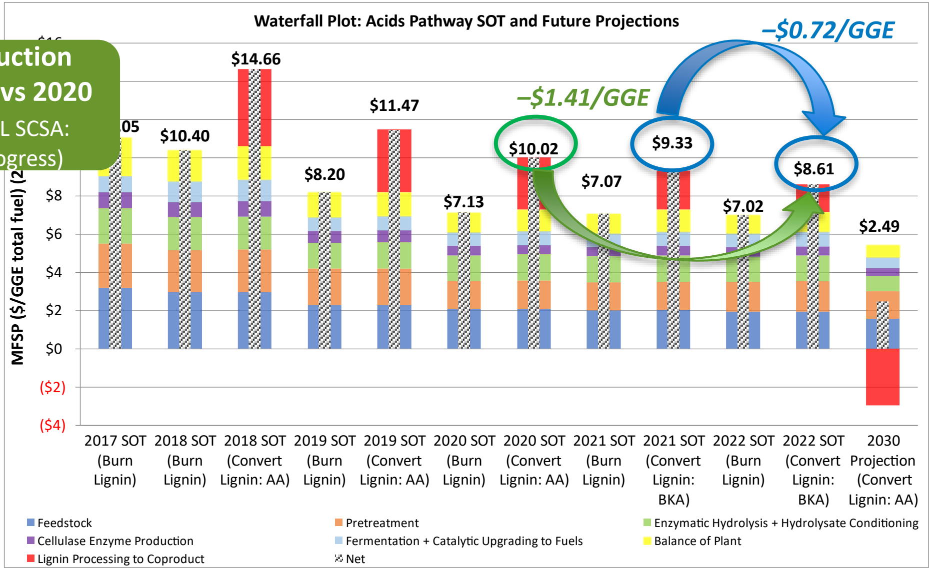


2. Progress and Outcomes

2022 SOT Achieves Further MFSP Advancements Across Value Chain

- 2022 SOT demonstrated further improvements in 2-stage deacetylation + EH
  - 89% glucan to glucose, 94% xylan to xylose, 70% arabinan to arabinose @ 10 mg/g enzyme loading
- BDO fermentation incorporated new arabinose-utilizing strain
  - >95% conversion of all three sugars to BDO (whole-slurry fermentation)
- Lignin conversion achieved further substantial improvements in lignin monomer fermentation to BKA
  - 1.58 g/g monomer yield (32% improvement) + 0.65 g/L-hr productivity (3X improvement)
- Overall translates to **$0.72-$1.05/GGE MFSP reduction ($0.67/GGE from lignin BKA improvements) vs 2021 SOT**

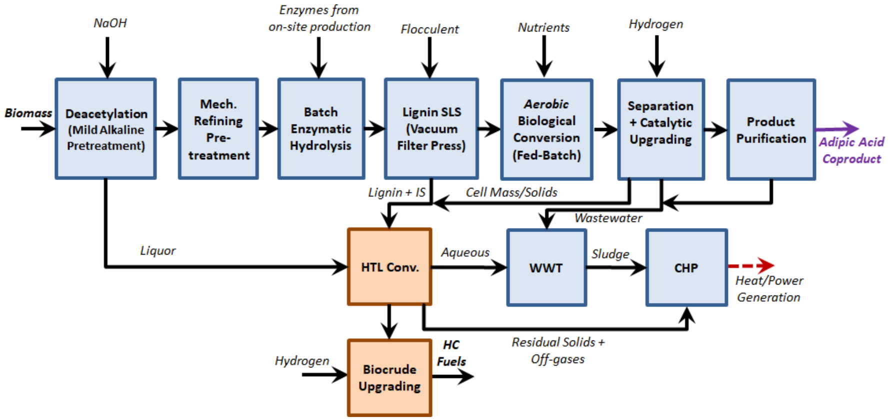


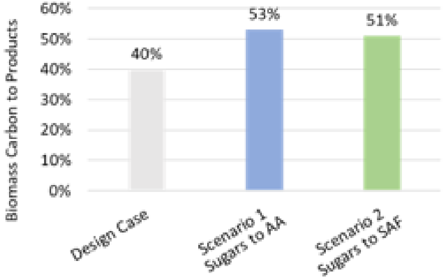


2. Progress and Outcomes

New Modeling Investigates Alternative Pathway Strategies: Hybrid BC/TC

- Evaluated several hybrid BC/TC routes as "alternative contingency" options
- BC: carbs → products (AA), TC: lignin → fuel (IDL)
  - Not found to offer promise: high capex/opex, low fuel yields (syngas diversion to drying wet lignin) = >$10/GGE MFSP
- BC: carbs → products (AA), TC: lignin → fuel (HTL)
  - More promising: comparable fuel yields, moderately higher MFSP ($0.74/GGE increase), 33% higher C efficiency
  - Also considered both carbs and lignin to fuels: significantly higher fuel yields >80 GGE/ton, but higher MFSP ($4/GGE)
  - Warrants further analysis moving forward





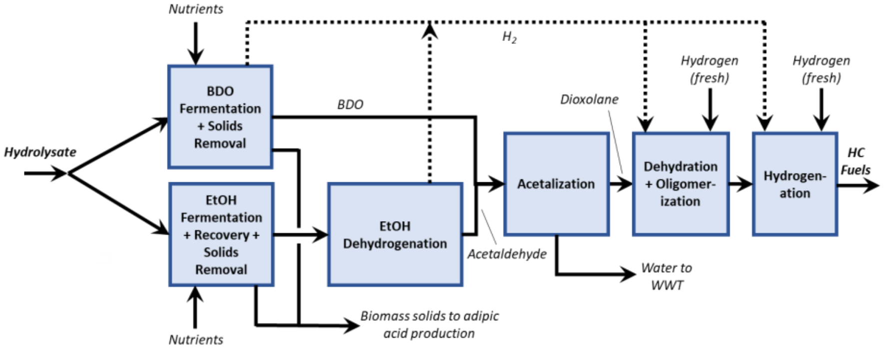
Joint analysis with PNNL 2.1.0.301

	2018 BDO Design Case	Base SAF (ETJ)	Adipic Acid/HTL Hybrid	SAF (ETJ)/HTL Hybrid
MFSP ($/GGE)	$2.47	$2.03	$3.21	$4.04
Fuel Yield (GGE/ton feed)	43.2	46.9	45.2	84.1

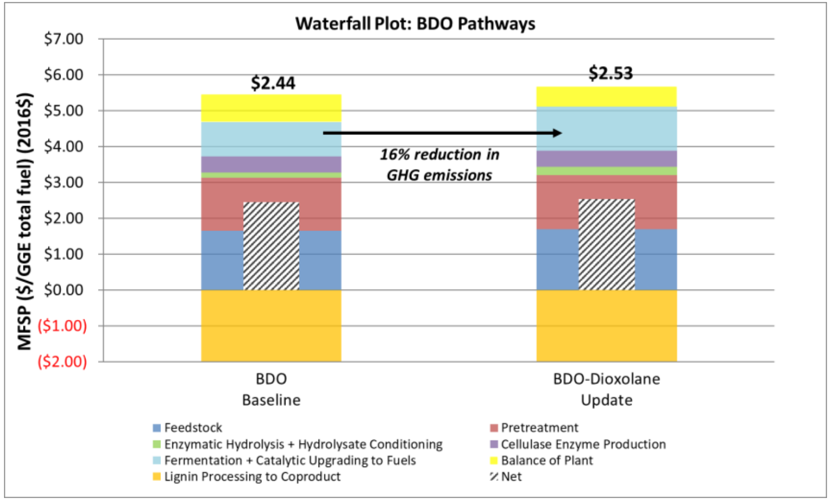
2. Progress and Outcomes

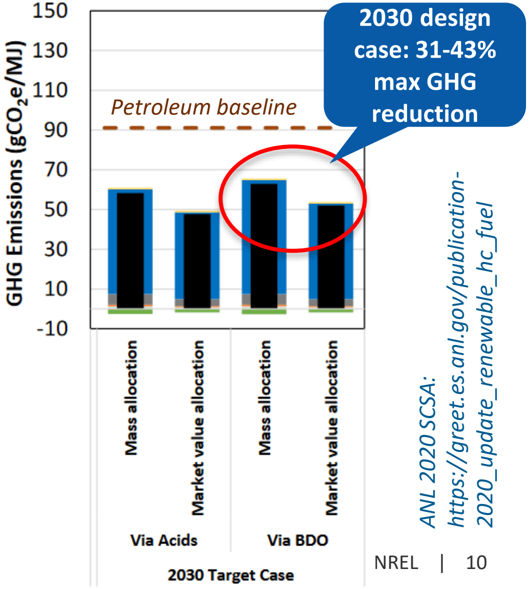
TEA Identifies BDO Pathway Optimization Opportunity (Integration with ChemCatBio CUBI + SepCon)

- BDO pathway presents promising potential for commercial deployment
- But, challenged by GHG reduction limits (<43%) below BETO goals (>70%)
  - Driven in part by high energy demands for aqueous BDO upgrading (90% water, 250 °C)
- New work under CUBI + SepCon investigating novel approach to purify BDO via dioxolane



- Dioxolane may be upgraded directly or reversed to BDO
- CUBI milestone (FY22 Q2) evaluated direct upgrading
- Found comparable MFSP (<5% difference) + 16% lower GHG potential
- Further evaluated under SepCon – *potential for even better results for MFSP + GHG via reactive extraction*



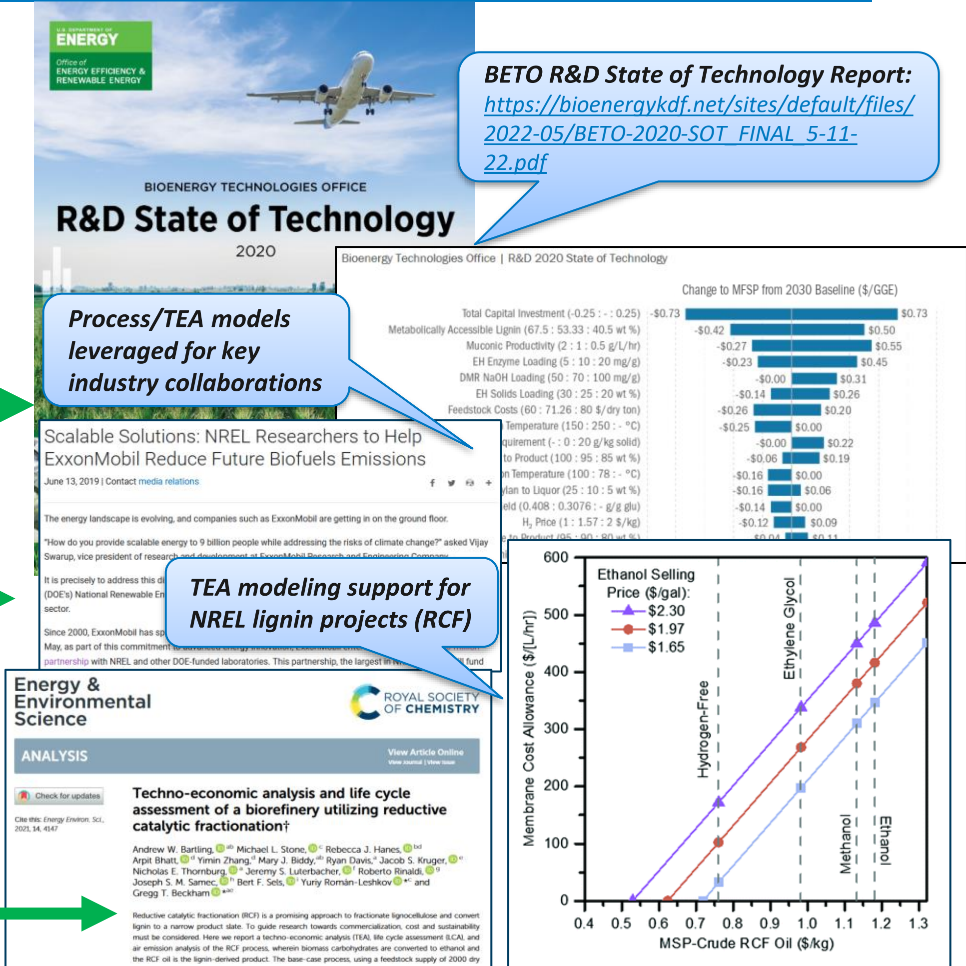


ANL 2020 SCSA: https://greet.es.anl.gov/publication-2020_update_renewable_hc_fuel

3. Impact

BC Analysis project provides high impact:

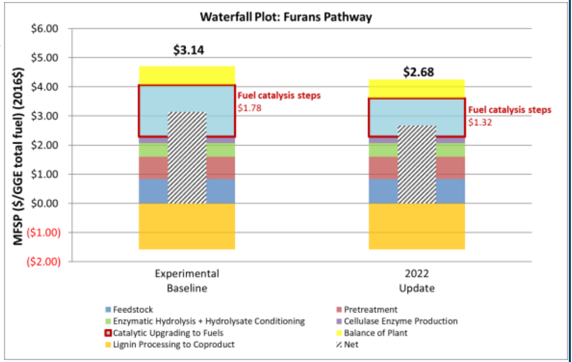
- Dissemination of information to the community:
  - **Over 22,000 downloads** of biochem TEA reports, 1,200+ downloads of TEA models in the **past 3 years** (https://www.nrel.gov/extranet/biorefinery/aspen-models/)
- Leverage framework set by this project to support a wide variety of stakeholders:
  - Research community, decision makers
  - **Guide R&D/DOE decisions to set targets**
  - Direct collaboration/participation with consortia
  - Industry/FOA collaborations
- Working to *prioritize further industry outreach* to guide next design report update (FY24):
  - Work with industry to **maximize commercial relevance of modeled designs for SAF production**
  - Revisit lignin processing approach based on newest high-impact R&D → RCF/Lignin-to-SAF



3. Impact

TEA paves the way for novel R&D concepts:

- **Support for ChemCatBio (CUBI) identifies promising new pathway via furans catalysis**
  - Key example utilizing this project for high-level TEA support to other BETO efforts
  - TEA highlights promising potential for direct sugar catalysis to SAF via furans: 40%+ higher fuel yield potential (no CO_2 loss), comparable or better MFSPs
  - Published NREL tech report, further work planned for FY23 with CUBI



https://www.nrel.gov/docs/fy21osti/80652.pdf

- **Support for CEH project highlights potential for maximizing enzyme efficiency**
  - NREL on-site enzyme model reflects "one" possible nth-plant scenario; may not reflect current industry costs for commercial enzyme sourcing
  - Continuous enzymatic hydrolysis (CEH) represents a novel approach/risk mitigation to maximize efficiency of enzymes
  - Sugar model TEA shows nearly 25% reduction in sugar selling price potential vs standard batch EH – to be further investigated with NREL CEH project

Minimum sugar selling price (cents/lb) – batch vs continuous EH	Batch EH (2019 SOT)	CEH (2022 update)	CEH (2023 update)	CEH (2023 update + 2X cycling)
1X enzyme cost ("nth-plant")	24.9	21.2	19.6	19.1
3X enzyme cost	29.7	25.4	21.4	20.1
10X enzyme cost	46.6	39.9	27.9	23.3

Summary

Biochemical Platform Analysis Provides Crucial Bridge From Technology R&D To Economics + Sustainability

Summary

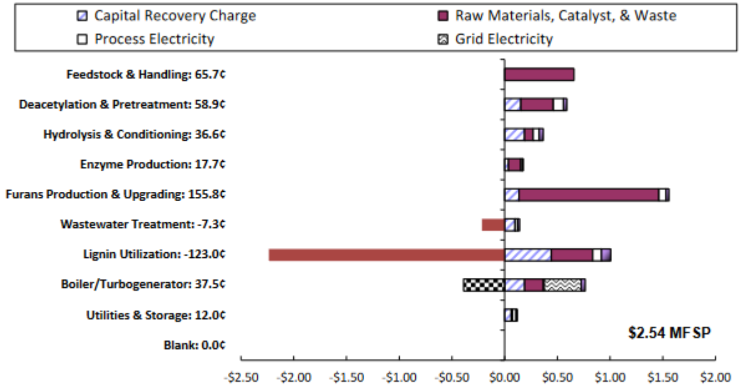
- **Management:** Strong team with **extensive collaboration** across BETO R&D portfolio + BETO analysis projects

- **Approach:** Continuous iteration of TEA concepts to **maximize efficiency of R&D dollars, de-risk** technology pathways

- **Impact:** High impact via **external engagement** (industry, research/consortia collaborators), focus on **transparent dissemination** of work

- **Outcomes:** Work is key to supporting BETO mission by **highlighting requirements to achieve economic + sustainability goals**, prioritize future research directions

- **Future Work:** Down-select leading integrated pathways to **maximize decarbonization + SAF potential with commercial relevance** for deployment (FY23 Go/No-Go) → Publish updated design report for selected pathways (FY24 milestone)



Quad Chart Overview

Timeline
- Project start date: Oct 1, 2022 (3-year cycle)
- Project end date: Sept 30, 2025 (3-year cycle)

	FY22 Costed	Total Award
DOE Funding	$500,000 (FY22 BA)	$1,500,000 (FY22-FY24)
Project Cost Share	N/A	N/A

TRL at Project Start: 3-5*
TRL at Project End: 4-6*
**TRL is N/A (Modality #5: strategic, market, and techno-economic analysis)*

Project Goal
Conduct techno-economic modeling and analysis to *quantify economic impact* of biochem platform R&D activities. This is done through creation of process/TEA models *relating key process parameters with overall economics and providing key outputs to quantify GHG emissions relative to BETO goals.*

End of Project Milestone
TEA/LCA quantification of opportunities and challenges for biochemical conversion of waste feedstocks (FY25 Q4): Beyond *design case updates for biochemical conversion of traditional herbaceous biomass feedstocks* during FY23-24, conduct preliminary TEA/LCA screening to *quantify tradeoffs between costs, GHG emissions, and fuel volume output* potential for biochemical conversion of at least one *waste feedstock material* (aqueous, solid, and/or gaseous). Deliver a milestone in technical report format for potential future publication documenting opportunities and challenges for waste feedstock processing relative to BETO goals.

Funding Mechanism
FY23 AOP Lab Call (Conversion)

Project Partners
No partners with shared funding (but collaborate frequently with other modeling/analysis projects at INL, ANL, PNNL; also provide TEA support to consortia for FCIC, ChemCatBio, SepCon, ABF)

Acknowledgements:

- Ling Tao
- Andrew Bartling
- Eric Tan
- Bruno Klein
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- Mike Himmel
- Mike Guarnieri
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- Tim Eggeman, Neoterics

Thank you! Questions?

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Acronyms

- AA = adipic acid
- BDO = 2,3-butanediol
- BKA = β-ketoadipate
- CUBI = Chemical Upgrading of Biological Intermediates (under ChemCatBio consortium)
- DMR = deacetylation and mechanical refining (pretreatment)
- Design case = future technical target projections to achieve TEA cost goals
- GGE = gallon gasoline equivalent
- LCA = life-cycle analysis
- M&E = material and energy (balances)
- MEK = methyl ethyl ketone
- MFSP = minimum fuel selling price
- OTR = oxygen transfer rate
- RCF = reductive catalytic fractionation
- SAF = sustainable aviation fuel
- SOT = state-of-technology (annual benchmarking to update TEA based on latest R&D data)
- TEA = techno-economic analysis

Additional Slides

Responses to Previous Reviewers' Comments

- Production costs, (set by the technology) offers a much more useful means of comparing competing routes, and is easier to present to a potential stakeholder. Yet in this presentation and most others, various forms of sales costs (set by the market, e. g., MFSP or the required sales price of adipic acid, sugars, BDO, etc.) are used for comparison.
- We would like to provide clarification that the TEA work conducted here in fact does solve for "production costs" as driven by the technology, based on underlying technology performance, yields, and associated capital/operating costs. This can then be compared against market values, e.g. MFSPs calculated from the TEA models can be compared to market values for fuels, which are currently set at a fixed $2.5/GGE basis per BETO guidance across all platforms. Any coproducts (such as adipic acid from lignin) are set at market value prices, typically based on historical multi-year market price averages, in determining resultant coproduct revenues they garner for the biorefinery.

- Impact enhancement by generating tools, as opposed to reports, could perhaps be of consideration. There are many skillful and competent members within this consortium that development of a block model TEA tool, for industrial applications, with discrete unit operation blocks tailored for a suite of processes, would be valuable and plausible. Acknowledging the challenges with TEA of novel technologies, which are not understood well at scale, well understood feed streams such as excess wet-mill, dry-mill, cane sugar capacity could be modeled for near term market impact.
- We have established several such tools over recent years for use by the public and industry partners. Two examples as mentioned briefly in the presentation include a public TEA sugar model (https://www.nrel.gov/extranet/biorefinery/aspen-models/, second set of files), as well as an Excel-based TEA tool to estimate the cost of biochemical intermediates over varying inputs for feedstock type, composition, cost, and conversion performance that does not require the use of Aspen (provided to an industry collaborator investigating opportunities for excess pulp mill capacity). We are also working to evaluate opportunities in the context of today's existing industry resources, for example to understand technology "bolt-on" possibilities to add cellulosic biomass processing capabilities to the front end of a Gen-1 facility (e.g. via DMR processing) and/or opportunities to switch to a new fermentation product with minimal redesign (e.g. 2,3-BDO).

- More information on the impact on $/GGE as a function of different balances between fuel and chemical production would be helpful. TEA should be flexible enough to move away from assuming that all carbohydrates will end up as fuel while lignin will supply chemical products to support the production of low value hydrocarbons.
- We thank the reviewer for this comment and agree. To address this, in FY22 we began further expanding the biorefinery configurations to also evaluate carbohydrates to products and lignin to fuels through several processing options. We plan to continue further expanding this assessment evaluating optimal TEA/LCA metrics for utilizing both the carbohydrate and lignin fractions for fuels and/or products as may be most practical for commercial deployment.

Publications, Patents, Presentations, Awards, and Commercialization

Publications/Reports (since 2021 review):

- B. Klein, I. McNamara, R. Davis, A. Mittal, D. Johnson, "Techno-economic assessment for the production of hydrocarbon fuels via catalytic upgrading of furans." NREL/TP-5100-80652. September 2021. https://www.nrel.gov/docs/fy21osti/80652.pdf
- R. Davis, A. Bartling, L. Tao, "Biochemical conversion of lignocellulosic biomass to hydrocarbon fuels and products: 2020 State of Technology and future research." NREL/TP-5100-79930. May 2021. https://www.nrel.gov/docs/fy21osti/79930.pdf
- R. Davis, A. Bartling, "Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2021 State of Technology and Future Research." NREL/TP-5100-82512. April 2022. https://www.nrel.gov/docs/fy22osti/82512.pdf
- H. Cai, L. Ou, M. Wang, R. Davis, A. Dutta, K. Harris, M. Wiatrowski, E. Tan, A. Bartling, B. Klein, D. Hartley, Y. Lin, M. Roni, D. N. Thompson, L. Snowden-Swan, Y. Zhu *(*report coordinated by ANL, contributions from BC Analysis)*. Supply Chain Sustainability Analysis of Renewable Hydrocarbon Fuels via Indirect Liquefaction, Ex Situ Catalytic Fast Pyrolysis, Hydrothermal Liquefaction, Combined Algal Processing, and Biochemical Conversion: Update of the 2020 State-of-Technology Cases. ANL technical report ANL/ESD-21/1 Rev 1. September 2021.
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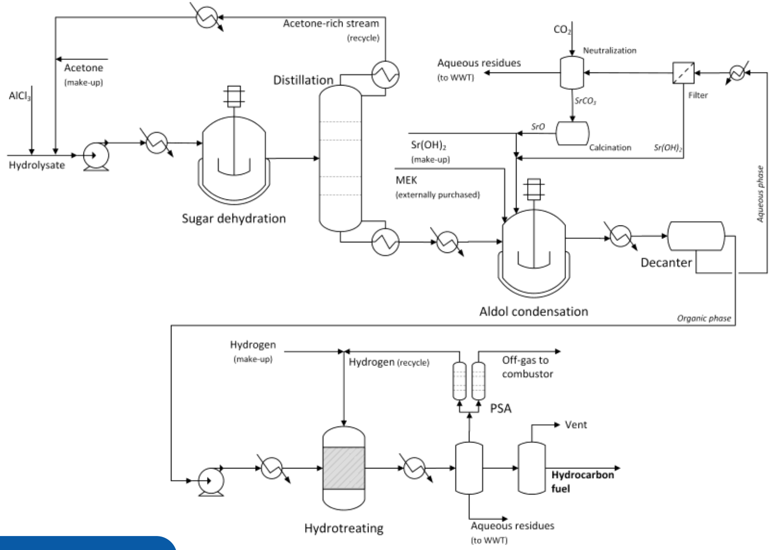
Backup Slides

Further Details: Furans Pathway (CUBI)

TEA Support for ChemCatBio (CUBI) Highlights Promising New Pathway via Furans

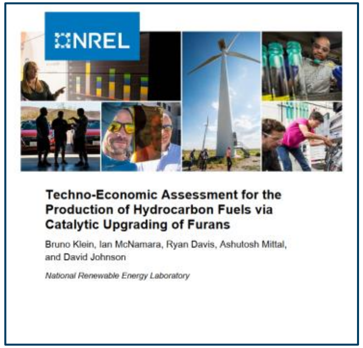
- BC Analysis project has provided TEA/LCA support for CUBI consortium 3+ years
- FY21-22: Investigated a novel pathway for direct sugar catalysis to fuels, published “mini-design report”
- Potential for comparable MFSPs, significantly higher fuel yields (minimal CO_2 production vs biological pathways = high C retention)
- More optimized approach (FY22) identified new solvent, better solvent recovery strategy, more optimal conditions = **~50% reduction in natural gas, further reduced MFSPs**
- Planning further work + LCA investigation in FY23



	Dedicated Biorefinery	Integrated Biorefinery
Feedstock rate	2,205 dry U.S. tons/day	
Online time	7,884 h/yr (90% online factor)	
Total fuel yield	108.4 GGE/dry U.S. ton feedstock	61.2 GGE/dry U.S. ton feedstock
Total fuel production rate	78.5 MM GGE/yr	44.3 MM GGE/yr
Adipic acid coproduct yield	284 lb/dry U.S. ton feedstock	276 lb/dry U.S. ton feedstock
Adipic acid production rate	205 MM lb/yr	200 MM lb/yr
Total variable OPEX excluding coproducts	$269 MM/yr	$187 MM/yr
Coproduct revenue	$193 MM/yr	$188 MM/yr
Total fixed OPEX	$20 MM/yr	$20 MM/yr
Total equipment cost	$414 MM	$416 MM
Total capital investment	$787 MM	$786 MM
TCI per annual gallon	$10.02/GGE	$17.75/GGE
Minimum Fuel Selling Price	**$2.54/GGE**	**$2.72/GGE**
Feedstock contribution	$0.66/GGE	$1.17/GGE
Fuel conversion contribution	$3.11/GGE	$3.71/GGE
Coproduct conversion contribution	−$1.23/GGE	−$2.16/GGE

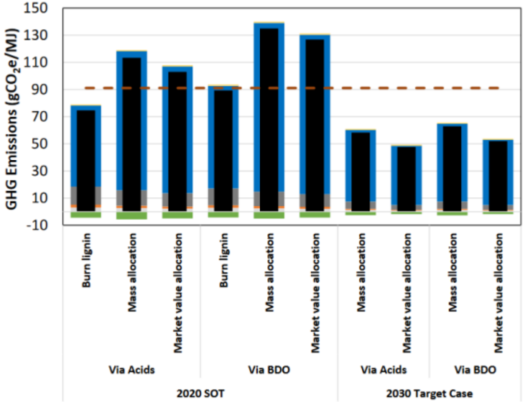
40+% higher vs biological design case pathways (43-45 GGE/ton)

FY22 improvements = ~$0.20/GGE further reductions (vs $2.49/GGE biological cases)

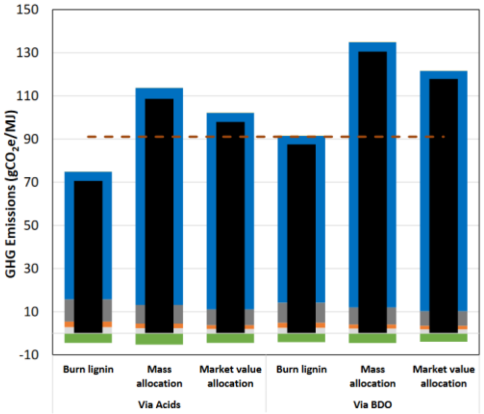


https://www.nrel.gov/docs/fy21osti/80652.pdf

Tracking LCA Metrics for SOTs: ANL SCSA Reports



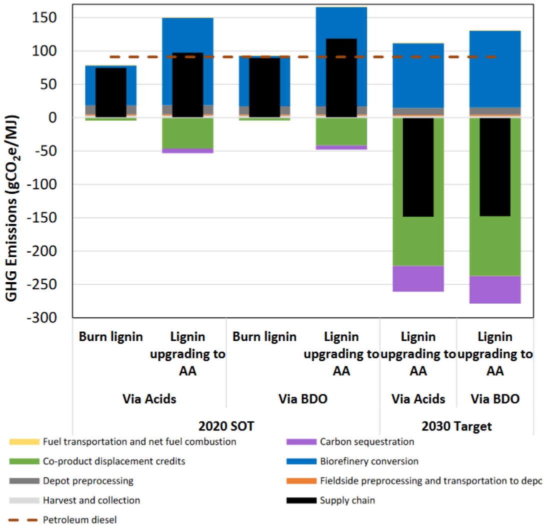
2020 SOT
https://greet.es.anl.gov/publication-2020_update_renewable_hc_fuel



2021 SOT
https://publications.anl.gov/anlpubs/2022/04/174410.pdf

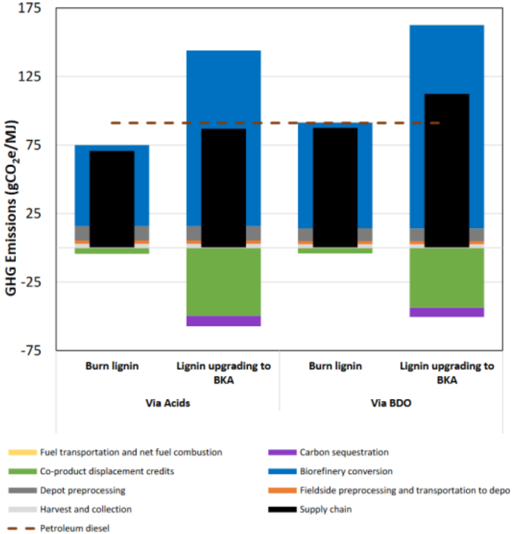
Process level allocation

5-7% fuel GHG reduction (market-value sub-allocation)



Displacement method

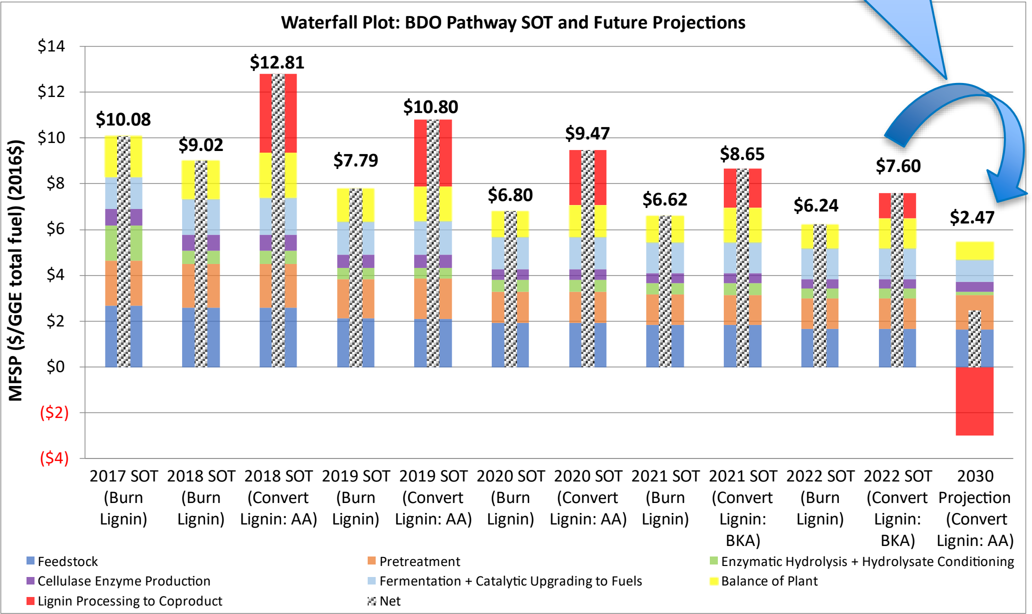
6-10% fuel GHG reduction

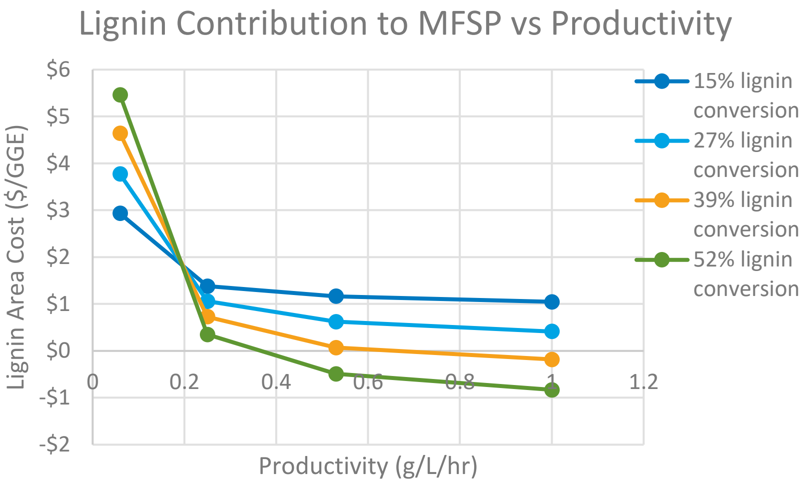


Lignin Drivers for 2030 MFSP Goals

R&D drivers for improved future MFSP:

- Increase sugar yields
- Reduce deacetylation loss
- Improve fermentation rates
- Lower catalysis costs
- **Improved lignin valorization performance**





- Lignin deconstruction/upgrading performance is key to meeting $2.5/GGE goals
- Productivity is primary cost driver particularly <0.2 g/L-hr (less sensitivity after 0.5 g/L-hr)
- Next, lignin conversion to monomers becomes key – break even at ~0.4 g/L-hr + 50% conversion or ~0.5 g/L-hr + 40% conversion