NREL
Transforming ENERGY

BETO 2021 Peer Review: 2.1.0.100 – Biochemical Platform Analysis

March 8, 2021

Biochemical Conversion & Lignin Upgrading Session

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Project Overview

Goal:

- Provide **process design and economic analysis support** for the biochemical conversion platform, to **guide R&D priorities towards economic viability**
  - Translate demonstrated/proposed research advances into economics (quantified as $/gal ($/GGE) selling price)

Outcomes:

- Heilmeier Catechism:
  - Aim: Assess cost-competitiveness and **establish process/cost targets** for biofuel production pathways
  - How done today: **Track progress** towards goals through state of technology (SOT) updates
  - Importance: Work to **prioritize research** – identify impact of key variables and design alternatives on overall economics, **disseminate** work transparently (“design report” process)
  - Risks: Need complex biorefineries to achieve fuel cost goals

Context:

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

Market Trends

Product
- Anticipated decrease in gasoline/ethanol demand; diesel demand steady
- Increasing demand for aviation and marine fuel
- Demand for higher-performance products
- Increasing demand for renewable/recyclable materials

Feedstock
- Sustained low oil prices
- Decreasing cost of renewable electricity
- Sustainable waste management
- Expanding availability of green H_2
- Closing the carbon cycle

Capital
- Risk of greenfield investments
- Challenges and costs of biorefinery start-up
- Availability of depreciated and underutilized capital equipment

Social Responsibility
- Carbon intensity reduction
- Access to clean air and water
- Environmental equity

NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Value Proposition

- This project is key to supporting the BETO mission by **highlighting requirements to achieve economic viability**, establishing and benchmarking progress towards goals

Key Differentiators

- **Iterative approach** – establish design case targets → refine TEA model details as process/research understanding evolves → focus in on key unit ops to guide R&D → update design case in synch with Platform
- Success is driven by **constantly re-evaluating optimization opportunities**, better R&D approaches for improving TEA

Quad Chart Overview

Timeline

- Project start date: Oct 1, 2019 (3-year cycle)
- Project end date: Sept 30, 2022 (3-year cycle)

	FY20	Active Project
DOE Funding	$500k (10/01/2019 – 9/30/2020)	$1.5 MM over current 3-year cycle (FY20-FY22)

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 under separate funding for FCIC, ChemCatBio, SepCon, Agile)

Barriers addressed

- Ct-D: Advanced Bioprocess Development
  - *Highlight cost drivers and priorities/tradeoffs between titers, rates, yields, bioreactor operation*
- At-E: Quantification of Economic, Environmental, and Other Benefits and Costs
  - *Perform cost/benefit analyses, quantify value proposition*

Project Goal

Conduct process and TEA modeling to support biochem platform R&D activities, relating key process parameters with overall economics. This is done by creating rigorous Aspen Plus models for conversion of herbaceous biomass to fuels and co-products, in order to relate key process parameters with overall economics and to track progress via SOT benchmarks towards BETO goals.

End of Project Milestone

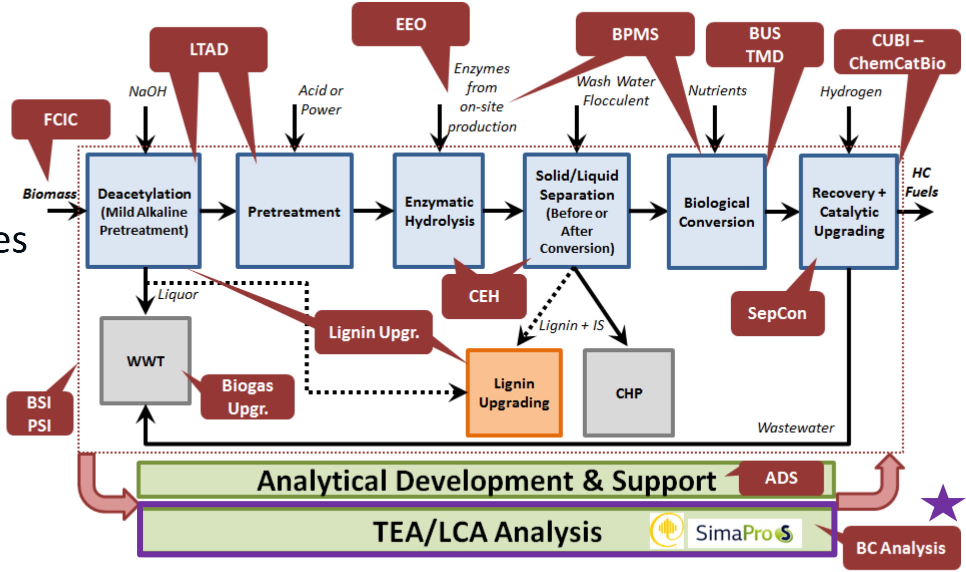
2022 Interim SOT demonstration and re-benchmarking: Deliver a 2022 SOT benchmarking update documenting achievement of NREL's Biochemical Platform 2022 MFSP goal (set based on FY21 Go/No-Go decision, at minimum 10% improvement relative to FY18 SOT benchmark), attributed to at least 5 experimentally-validated data metrics for at least one pathway approach. The outcomes will inform a re-benchmarking assessment to highlight key remaining gaps and risks that must be addressed in the baseline design case configuration or otherwise propose a new configuration for consideration moving into the next 3-year cycle.

Funding Mechanism

Direct AOP funding

1. Management

- This project is **highly integrated with research efforts**, assist in key R&D planning across Platform:
  - Platform structure = TEA interaction with all projects
  - Interface with multiple consortia tie-ins (FCIC, SepCon, ABF, CUBI, Co-Optima) – iterate to solve key issues
- 4 process engineers, strong biochem TEA capabilities
- Risk identification/mitigation:
  1) Optimizing only for TEA at the expense of LCA
     - Mitigation: Work closely with ANL partners to **foster information exchange**, relay LCA drivers to researchers for co-optimization alongside TEA
  2) Premature down-selection to an infeasible pathway
     - Mitigation: Keep "all eggs out of one basket", **continuously re-assess** base case framework against alternative approaches and new concepts



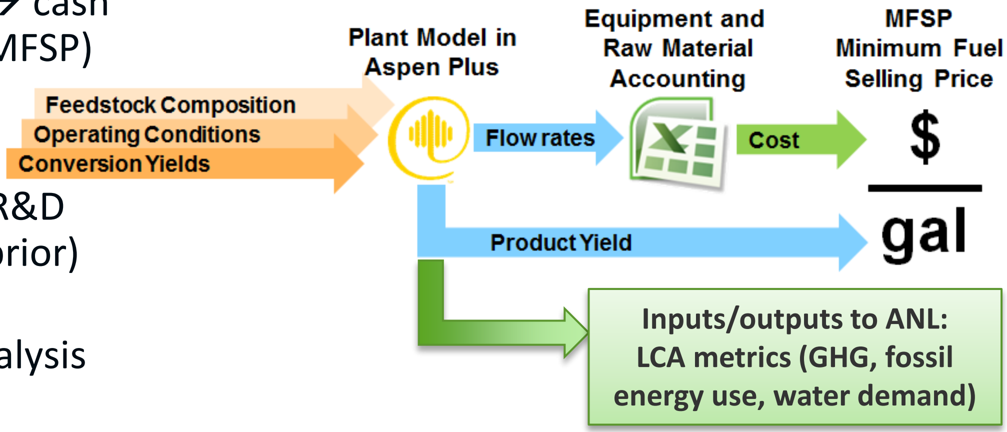
- **Prioritize dissemination** of TEA through reports, conference talks
- Project management tracked via milestones

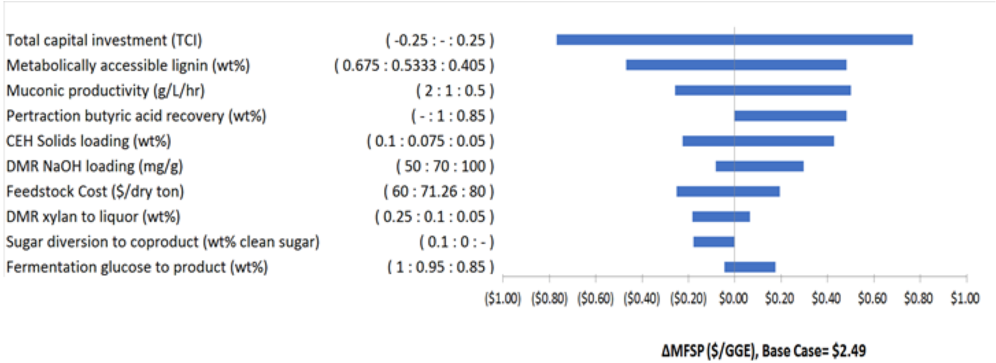
Project Milestones/Activities	FY19 Q1	FY19 Q2	FY19 Q3	FY19 Q4	FY20 Q1	FY20 Q2	FY20 Q3	FY20 Q4	FY21 (planned) Q1	FY21 (planned) Q2	FY21 (planned) Q3	FY21 (planned) Q4
Base Case Model Optimization/Benchmarking Updates												
Feedstock compositional impacts in conversion TEA					▼							
2-stage deacetylation via sodium carbonate pre-extraction						▼			▼			
TEA screening for deacetylation NaOH recovery								▼				
Out-year platform cost projections										●		
SOT benchmarking	▲			▲					▲			▲
Screening for Alternative Process Configurations												
TEA assessment for lignin RCF/alternative lignin processing		▼					▼				▼	
Alternative lignin coproduct analysis			▼									
Biogas upgrading opportunities			▼									

▲ = Milestone ▼ = Quarterly progress measure ● = Go/no-go decision

2. 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
- Challenges:
  - More difficult to develop representative models for new/novel technologies that are not yet well-understood at scale
    - Solicit **engineering subcontractor support** to refine models/design details
  - Building credible TEA projections as supporting data is still being developed
    - Frequent communication with researchers to set "theoretical potential" limits up front, refine models as data catches up
    - **Stage-gate decision points** to avoid making assertions without supporting data (example: **Go/No-Go** on out-year TEA projections considering status of data availability)



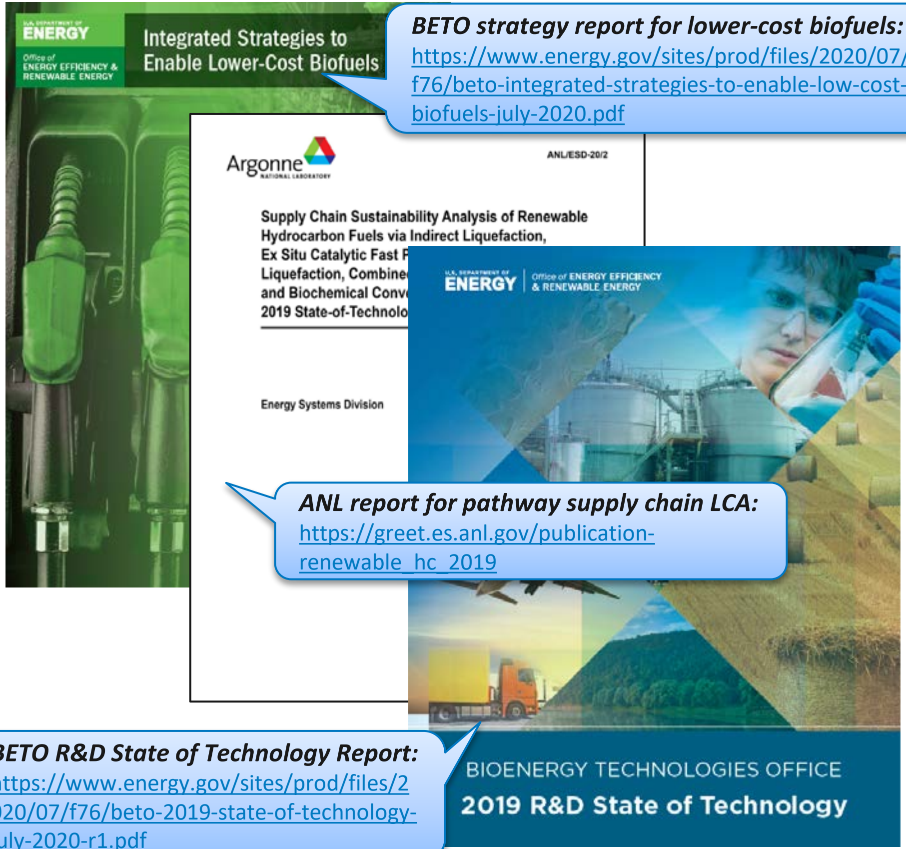


3. Impact

TEA modeling provides high impact:

- Analysis serves a wide variety of stakeholders
  - *Industry (inform decisions, solicit guidance)*
    - *Ex #1: Industry subcontract to improve TEA fidelity for pertractive membrane recovery of acids*
    - *Ex #2: Leveraging TEA for CRADA/FOA support*
  - *Research community, decision makers*
  - *Identify **opportunities for near-term market impact***
    - *Ex: TEA tool (Excel) supplied to industry to estimate sugar costs from excess pulp mill capacity*
- **Guides R&D, DOE decisions, sets out year targets**
  - *Technical targets, e.g.:*
    - *Deconstruction: enzyme loadings, NaOH usage (LTAD)*
    - *Fermentation: process yields, productivities (BSI/BUS)*
    - *Upgrading: catalyst type, WHSV, lifetime (CUBI)*
    - *Lignin: conversion/upgrading yields (Lignin Upgr.)*
  - *Cost targets (BETO goal: <$2.5/GGE MFSP by 2030)*
- **Prioritize dissemination** of information through tech reports, models: *https://www.nrel.gov/extranet/biorefinery/aspen-models/*
  - ***~16,000 downloads** of TEA reports **(past 3 years)***

TEA outputs leveraged for other high-visibility reports:



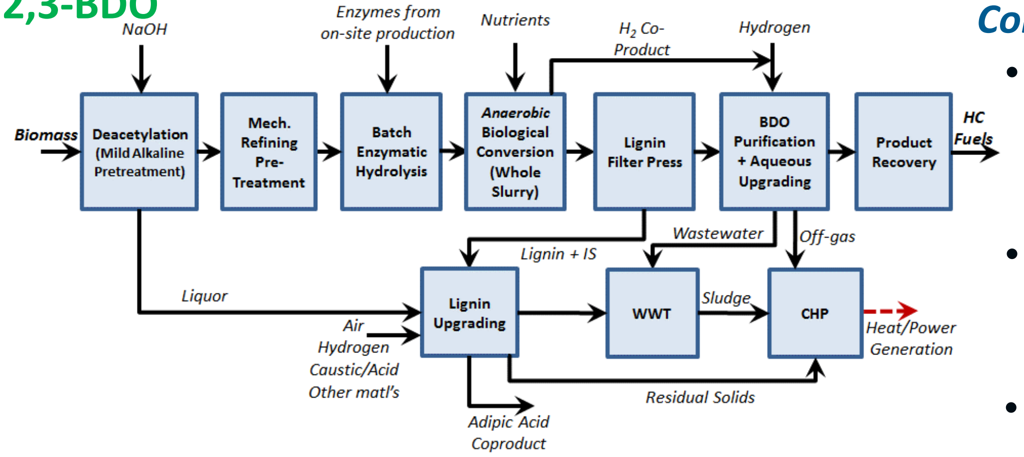
BETO strategy report for lower-cost biofuels: https://www.energy.gov/sites/prod/files/2020/07/f76/beto-integrated-strategies-to-enable-low-cost-biofuels-july-2020.pdf

ANL report for pathway supply chain LCA: https://greet.es.anl.gov/publication-renewable_hc_2019

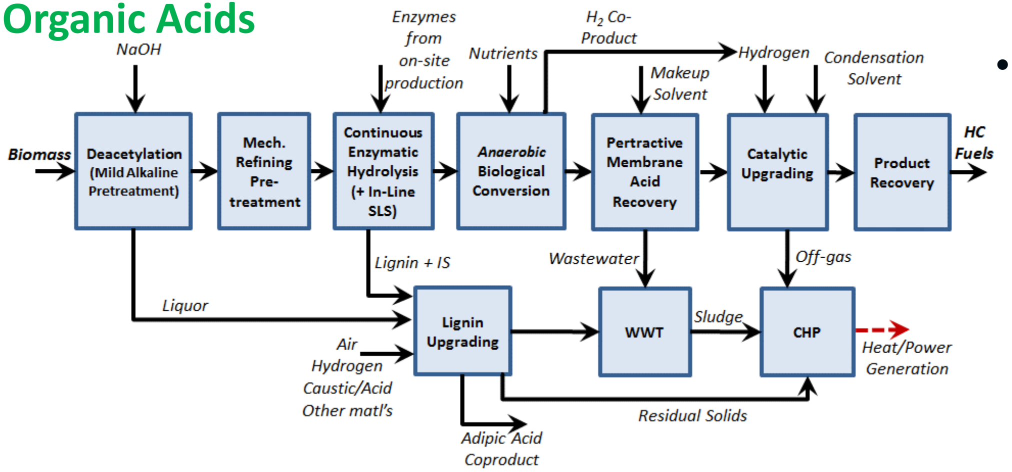
BETO R&D State of Technology Report: https://www.energy.gov/sites/prod/files/2020/07/f76/beto-2019-state-of-technology-july-2020-r1.pdf

4. Progress and Outcomes

2,3-BDO

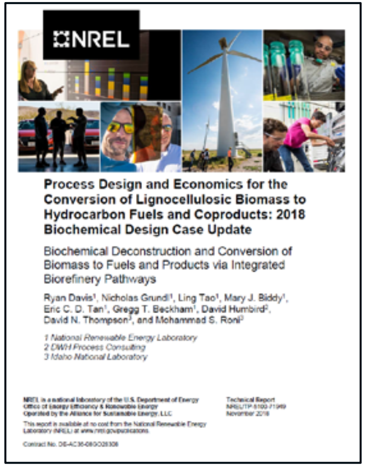


Organic Acids



Context: Pathways Investigated Under BC Platform

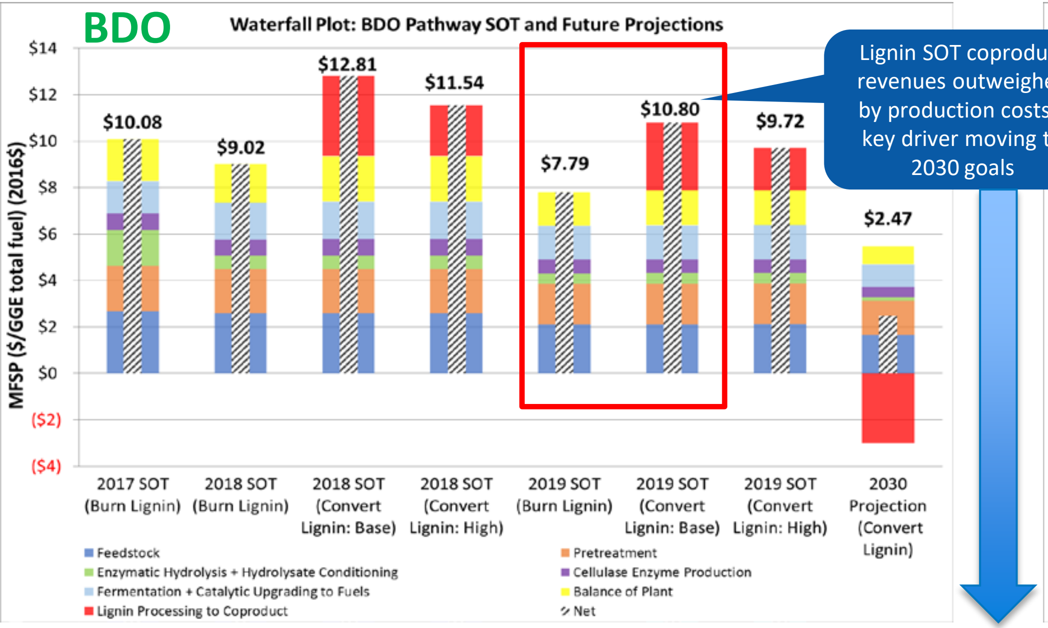
- Two pathways investigated, per 2018 NREL "design report":
  - 2,3-BDO to fuels
  - C4 acids to fuels
- Both pathways include lignin deconstruction + upgrading to coproducts (adipic acid as example)
- BDO: Batch EH + whole-slurry fermentation, aqueous upgrading
- Acids: Continuous EH (w/ solids removal),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

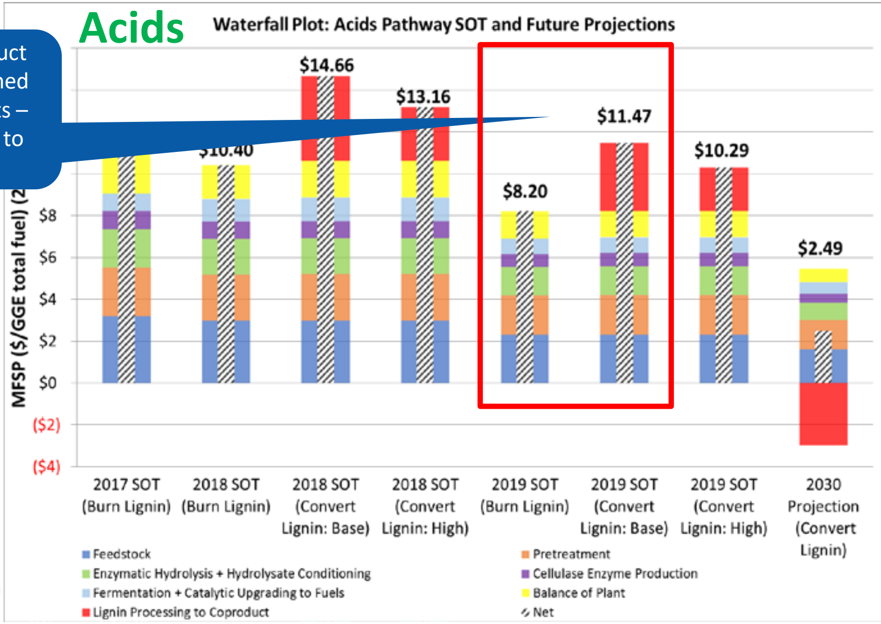


https://www.nrel.gov/docs/fy19osti/71949.pdf

4. Progress and Outcomes

2019 SOT Benchmarking Highlights Improvements, Drivers, Gaps



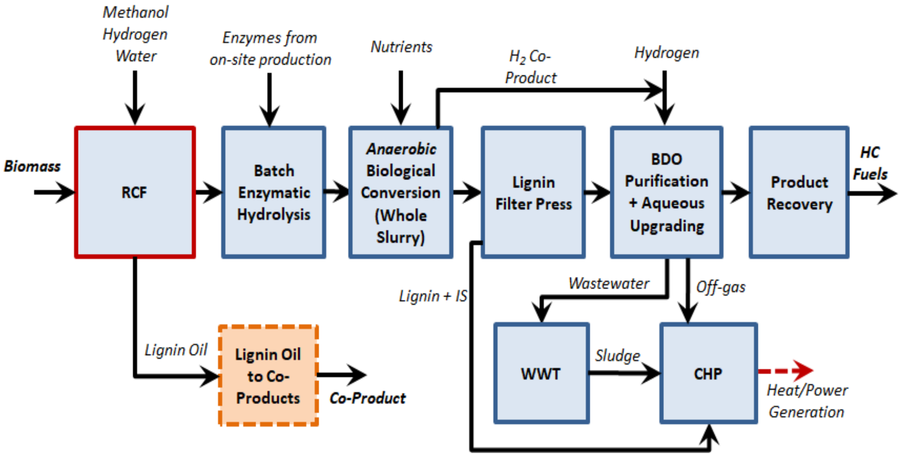


- **2019 SOT: $1.2 – $2/GGE reduction in MFSP**, enabled by higher sugar + fermentation yields
- But, two primary challenges remain for the BC pathway moving forward:
  - TEA: **Lignin coproduct train performance** (deconstruction yield + fermentation productivities) = largest gaps between SOT vs targets
  - LCA: Substantial GHG emissions attributed to DMR pretreatment (**NaOH demands** constitute single largest chemical LCA burden via chlor-alkali synthesis)

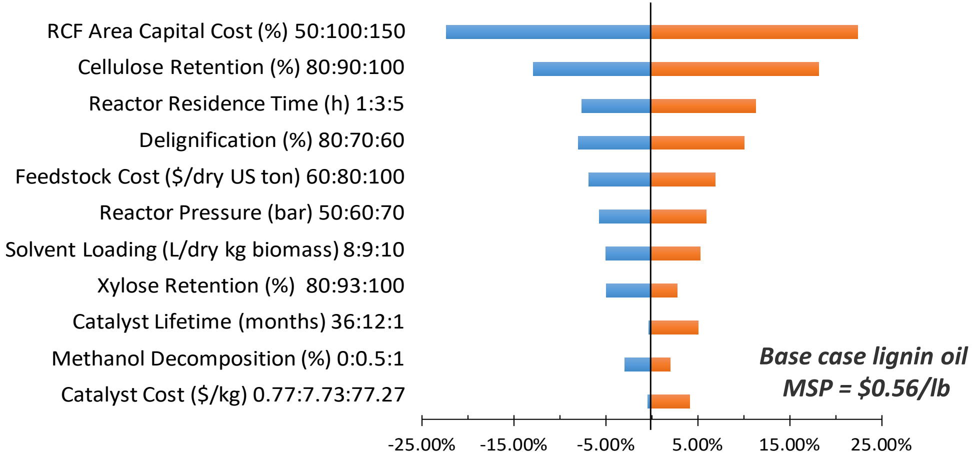
4. Progress and Outcomes

Alternative Lignin "Contingency Strategies" Highlight Additional Paths to $2.5/GGE

- Given strong MFSP dependence on lignin coproducts, **new paths also being considered** beyond SOT approach
- TEA evaluated alternative process via reductive catalytic fractionation (RCF); in collaboration with Lignin First (2.2.3.106)
- Incorporated RCF as alternate pretreatment operation, solubilizing lignin oil (*methanol/H_2 solvolysis + catalysis*) while leaving carbs-to-fuels



- Estimated **$0.56/lb lignin oil selling price** required to be valorized as a coproduct to maintain $2.5/GGE MFSP
- Strong dependence on RCF reactor capex (residence time, pressure, solvent loading)
- Highlighted **key opportunity for higher-boiling solvent** to reduce reactor pressure/lignin MSP
- Further TEA/LCA improvements via membranes

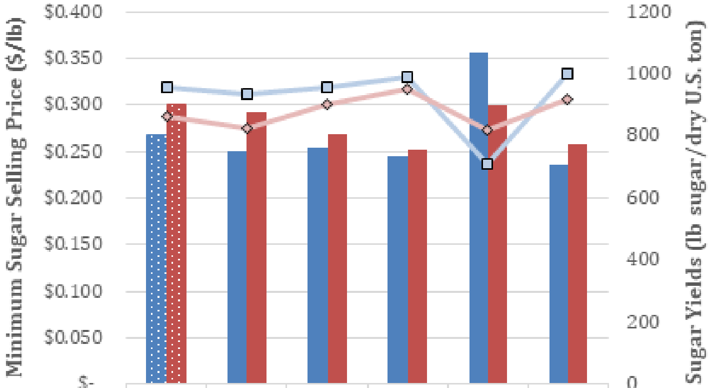


4. Progress and Outcomes

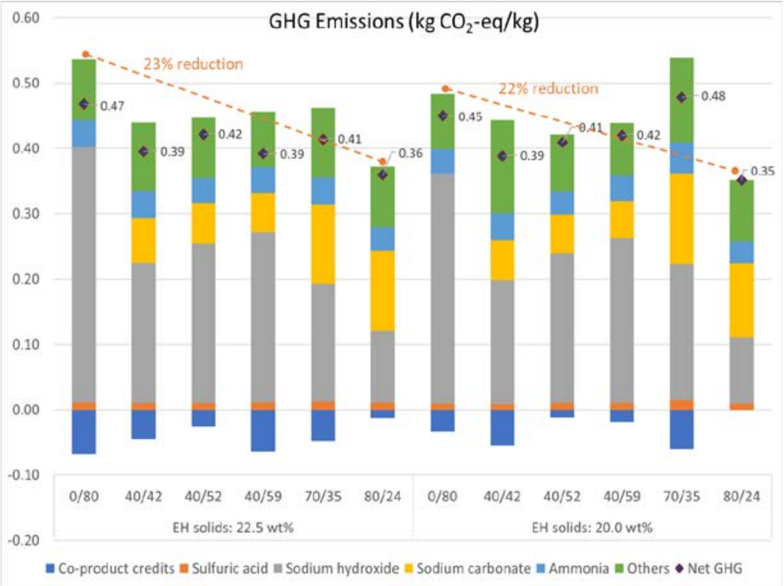
Addressing LCA Challenges for Deacetylation NaOH – Solution: Replace NaOH

- LTAD moved to **2-stage deacetylation with Na_2CO_3** pre-extraction to reduce NaOH loading
- Na_2CO_3 = 1/3 GHG and cost of NaOH
- TEA/LCA incorporated data across 12 scenarios using sugar model
- Optimal case identified at **80 kg Na_2CO_3 + 24 kg NaOH** per tonne biomass = **12% lower sugar cost, 22% lower GHGs**

	LCA metrics per ANL's Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model		TEA metrics used in NREL modeling
	GHG (kg CO_2e/kg)	Total Energy (MJ/kg)	Chemical Cost ($/lb)
NaOH (100%)	2.0	32.3	0.24
Na_2CO_3 (100%), excluding decomposed CO2	0.7	5.94	0.08



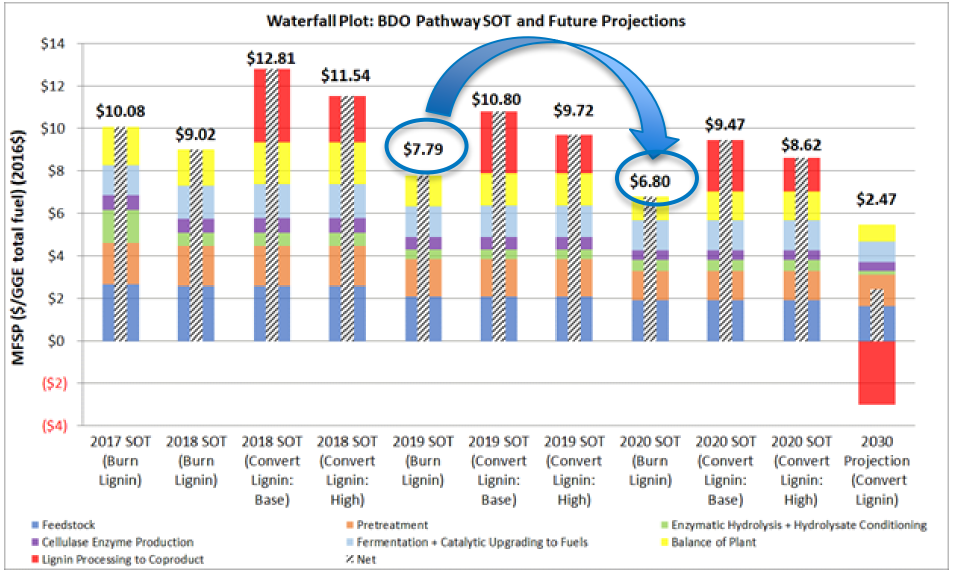
	0/80	40/42	40/52	40/59	70/35	80/24
MSSP, 20.0% solids EH	$0.268	$0.251	$0.254	$0.245	$0.356	$0.235
MSSP, 22.5% solids EH	$0.300	$0.292	$0.269	$0.252	$0.300	$0.258
Sugar Yield, 20.0% solids EH	957	934	955	988	709	1001
Sugar Yield, 22.5% solids EH	862	826	901	953	819	920

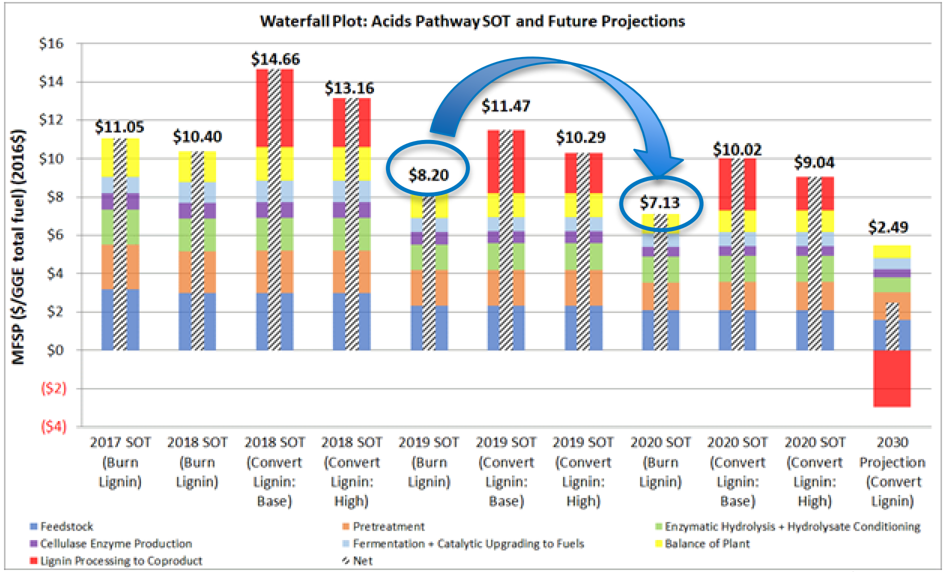


4. Progress and Outcomes

2020 SOT Updates Demonstrate Impact of 2-Stage DMR

- 2020 SOT incorporated data for new 2-stage DMR approach – led to **~$1/GGE MFSP reductions** beyond 2019 SOT for lignin combustion base cases
- Reflects favorable hydrolysis yields **(88% glucose, 93% xylose) at 10 mg/g enzyme loading**
- Most fuel train targets now approaching 2030 goals (10 years early) – future work will re-evaluate to increase future target performance further
- LCA in progress (collaborating with ANL partners)

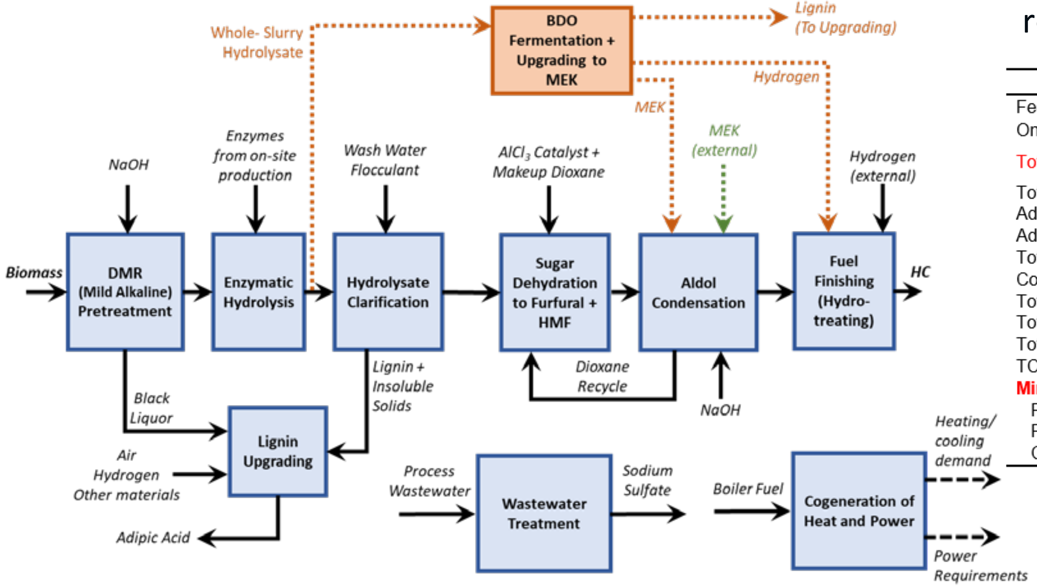




4. Progress and Outcomes

Collaboration with ChemCatBio Establishes Potential for New Sugar Catalysis Pathway

- Provided TEA support for ChemCatBio (CUBI) to investigate new fuel pathway via **sugar catalytic upgrading**
- Pathway focuses on sugar dehydration to furans, aldol condensation via ketone addition, hydrotreating – yields C14-16 HC fuels
- Investigated ketone sourcing via (a) *in situ* production from sugars, (b) externally purchased MEK



- Projected MFSPs at \$2.58/GGE for dedicated pathway (purchased MEK), \$2.74/GGE for integrated pathway (*in situ* MEK)
- **Very high fuel yields** at 61 GGE/ton biomass (integrated pathway) = **~40% higher than BDO/acids design case** pathways (no CO_2 rejection = high C efficiency to fuels)
- But, tradeoffs in high energy demands for solvent use + recovery, higher capex/opex costs

	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 coproduct[a]	\$269 MM/yr	\$186 MM/yr
Coproduct revenue	\$192 MM/yr	\$188 MM/yr
Total fixed OPEX	\$20 MM/yr	\$20 MM/yr
Total equipment cost	\$420 MM	\$419 MM
Total capital investment (TCI)	\$797 MM	\$791 MM
TCI per annual gallon	\$10.15/GGE	\$17.86/GGE
Minimum Fuel Selling Price	**\$2.58/GGE**	**\$2.74/GGE**
Feedstock contribution	\$0.66/GGE	\$1.17/GGE
Fuel conversion contribution	\$3.15/GGE	\$3.73/GGE
Coproduct conversion contribution	-\$1.23/GGE	-\$2.16/GGE

[a] Excludes coproduct revenue from sale of adipic acid and sodium sulfate (next row). Not including catalyst replacement schedules.

Summary

Category	Market need
Product	Anticipated decrease in gasoline/ethanol demand; diesel demand steady
Product	Increasing demand for aviation and marine fuel
Product	Demand for higher-performance products
Product	Increasing demand for renewable/recyclable materials
Feedstock	Sustained low oil prices
Feedstock	Decreasing cost of renewable electricity
Feedstock	Sustainable waste management
Feedstock	Expanding availability of green H_2
Feedstock	Closing the carbon cycle
Capital	Risk of greenfield investments
Capital	Challenges and costs of biorefinery start-up
Capital	Availability of depreciated and underutilized capital equipment
Social Responsibility	Carbon intensity reduction
Social Responsibility	Access to clean air and water
Social Responsibility	Environmental equity

NREL's Bioenergy Program Is Enabling a Sustainable Energy Future by Responding to Key Market Needs

Summary

- **Management:** Strong team with **extensive collaboration** across internal + consortia R&D work
- **Approach:** Continuous iteration of TEA concepts to **maximize efficiency of R&D dollars**
- **Impact:** High impact via **external engagement** (industry, research collaborators), focus on **transparent dissemination** of work
- **Outcomes:** Work is key to supporting BETO mission by **highlighting requirements to achieve economic viability**, benchmarking progress towards goals

Future Work

- TEA for out-year targeting **(Go/No-Go)** decision to establish **future projections to achieve 2030 goals**
- TEA/LCA assessment for **alternative lignin/ biorefinery configurations**, evaluating cost + GHG tradeoffs for further "contingency strategy" options
- End-of-cycle SOT and re-benchmarking to **demonstrate 2022 MFSP goals, highlight gaps or propose new pathway designs** for next AOP cycle

Acronyms

- BDO = 2,3-butanediol
- 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
- M&E = material and energy (balances)
- MEK = methyl ethyl ketone
- MFSP = minimum fuel selling price
- MYP = BETO's Multi-Year Plan (formerly MYPP = Multi-Year Program Plan)
- OTR = oxygen transfer rate
- RCF = reductive catalytic fractionation
- SOT = state-of-technology (annual benchmarking to update TEA based on latest R&D data)
- TEA = techno-economic analysis

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Thank you!
Questions?

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Additional Slides

Responses to Previous Reviewers' Comments

- This project provides process designs and economic analysis for many existing BETO projects. This analysis is then used to identify worthwhile projects, in particular helping identify go/no-go decision points. A key success of this analysis is the identification of two promising processes (2,3-BDO and organic acids) and to deemphasize aerobic processes focused on fatty alcohol production. Overall, the team is making excellent process and addresses a key need within the BETO portfolio. The project would benefit from more input from industry and an increased focus on the costs of product recovery, which will influence upstream design decisions.
- We thank the reviewers for their positive feedback in recognizing the impact of this project for BETO and the utility in guiding R&D priorities for NREL and the community. We welcome the suggestions to increase collaborations with and feedback from industry to help refine the TEA models, particularly for more new/novel process operations including key separation and product recovery steps. Two such mechanisms for this include subjecting our draft design reports to a thorough peer review vetting process (including stakeholders from industry), and subcontracting with engineering firms or other expert consultants to improve process understanding for such operations. For example, since the 2019 peer review we have recently completed a subcontract with one such consultant from industry (Neoterics) to improve current design and cost estimates for carboxylic acid product recovery via membrane pertraction, to be incorporated into future TEA model iterations. Additionally, this project works closely with ongoing efforts under the Separations Consortium to share information and further improve the fidelity for such separations processes.

- Ideally, feedback to the various experimental groups could be provided on a faster basis. Obviously, this is a question of resources. Nonetheless, the modeling work is a critical component to many projects.
- Yes, to the extent our resource availability and timing allows, we seek to support as many projects under the portfolio as possible (both internal and external to NREL), but bandwidth is indeed a limitation which requires identifying priorities and staging TEA support activities over time. Recognizing the time burdens for in-depth TEA modeling, when possible we have also provided less-granular TEA outputs on a higher level, i.e. by recycling previous models with similar or overlapping operations and truncating the boundary to an intermediate product (rather than extending out through final product recovery and upgrading) with more qualitative discussion on potential ramifications for downstream processing. We have also supported other NREL analysis projects to investigate the development of more rapid turn-around TEA tools for higher-level feasibility assessment.

Publications, Patents, Presentations, Awards, and Commercialization

Publications/Presentations (since 2019 review):

- R. Davis, N. Grundl, L. Tao, M.J. Biddy, "2018 NREL design report: Integrated biorefinery pathways for biochemical conversion of biomass to hydrocarbon fuels and bio-products – Process design and techno-economics." 2019 Symposium on Biotechnology for Fuels and Chemicals, May 1, 2019, Seattle, WA.
- R. Davis, A. Bartling, L. Tao, "Biochemical conversion of lignocellulosic biomass to hydrocarbon fuels and products: 2019 State of Technology and future research." NREL/TP-5100-76567, April 2020. https://www.nrel.gov/docs/fy20osti/76567.pdf
- Joint contributions from 2.1.0.100 (Biochemical Platform Analysis), 2.1.0.302 (Thermochemical Platform Analysis), 4.1.1.30 (Strategic Support), and collaborations with other partners from ANL, INL, PNNL, ORNL: "Integrated Strategies to Enable Lower-Cost Biofuels." DOE Technical Report, July 2020: https://www.energy.gov/sites/prod/files/2020/07/f76/beto-integrated-strategies-to-enable-low-cost-biofuels-july-2020.pdf
- H. Cai, L. Ou, M. Wang, E. Tan, R. Davis, A. Dutta, L. Tao, D. Hartley, M. Roni, D. Thompson, L. Snowden-Swan, Y. Zhu *(report coordinated by ANL)*. "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 2019 State-of-Technology cases." ANL technical report, April 2020. https://greet.es.anl.gov/publication-renewable_hc_2019
- S.P. Adhikari, J. Zhang, Q. Guo, K.A. Unocic, L. Tao, Z. Li *(joint with ChemCatBio).* A hybrid pathway to biojet fuel via 2, 3-butanediol. *Sustainable Energy & Fuels.* 2020, 4: 3904-3914.

Backup Slides

4. Progress and Outcomes

Addressing LCA Challenges for Deacetylation NaOH – Solution #2: Recycle NaOH

- Conducted TEA joint with LTAD project to evaluate NaOH recycling options: Kraft, MET, ED
- Kraft indicated some potential, but not a preferred strategy as it burns lignin in black liquor
- MET recycling demonstrated the potential for **6.5% MSSP reduction** vs 6% increase for ED recycling (driven by ~10X higher NaOH recovery via MET, higher energy efficiency)
- Driven by achievable current density – requires 5-10 mA/cm^2 for viability (current SOT values ≤ 1 mA/cm^2 – likely a longer-term strategy)

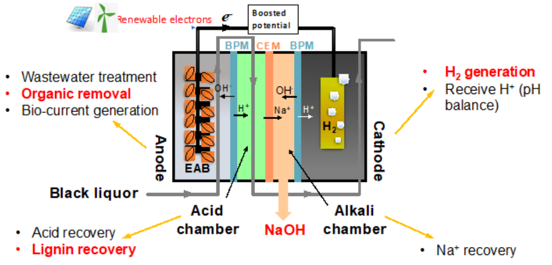
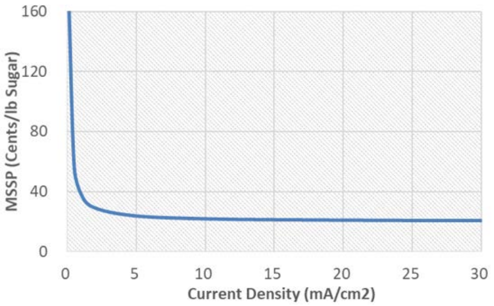
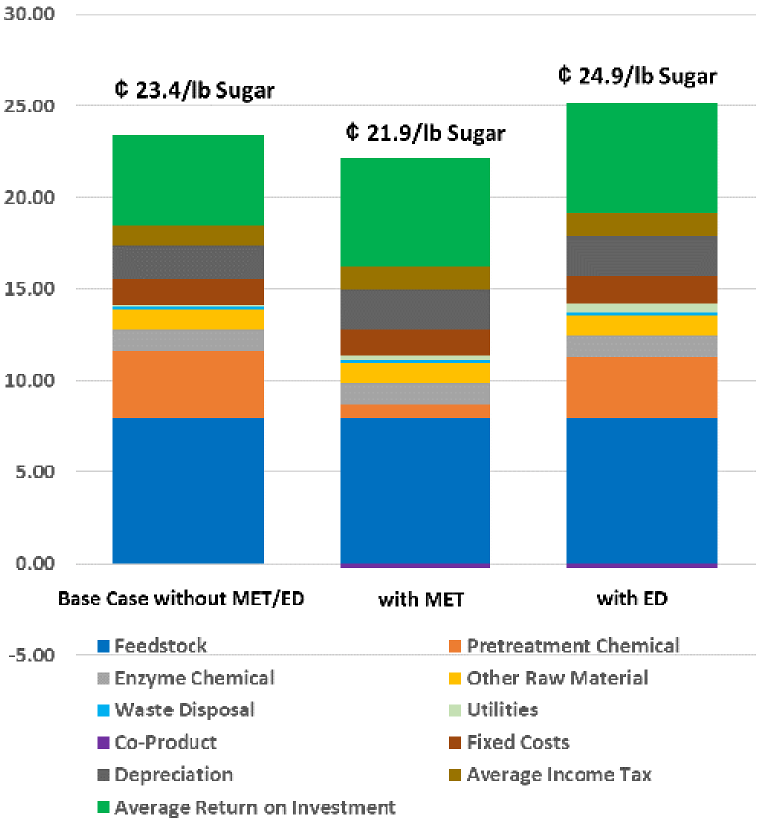
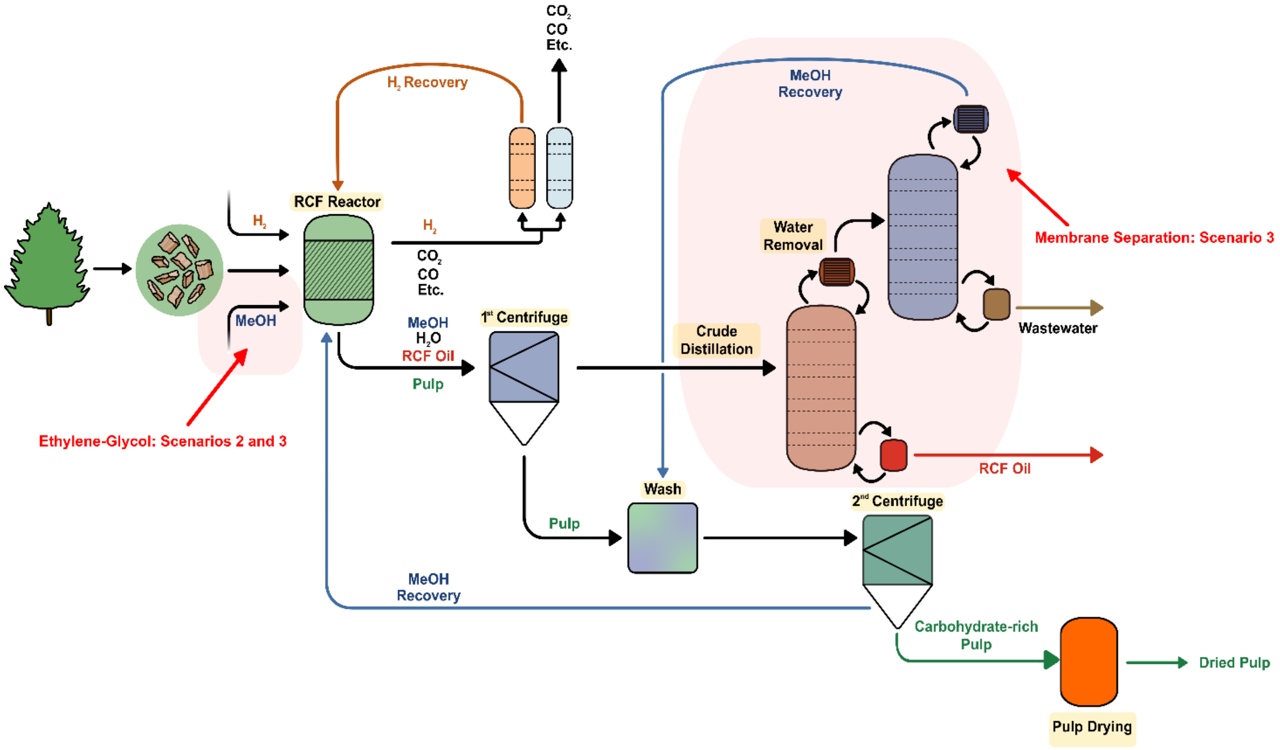


Diagram credit: Xiaowen Chen





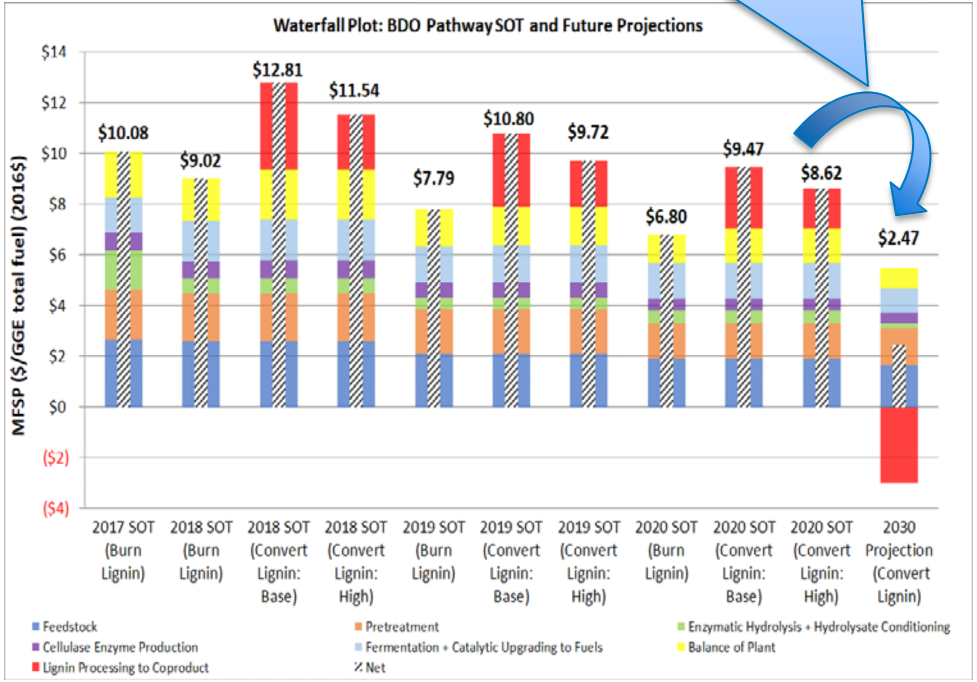
RCF Processing (Lignin-First)

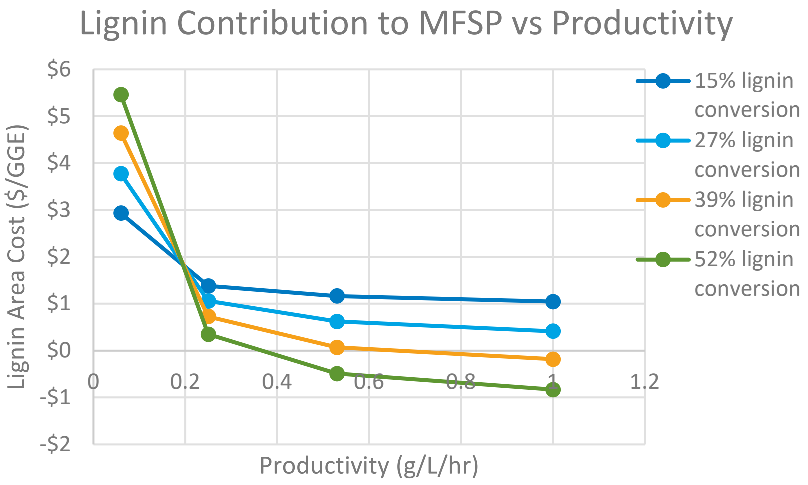


Path Forward to 2030 MFSP Goals

R&D drivers for improved future MFSP:

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





- Moving forward, lignin deconstruction/upgrading performance will be key to meeting $2.5/GGE goals
- Primary emphasis on improving productivity first to >0.2 g/L-hr (less sensitivity after 0.5 g/L-hr)
- Next, lignin conversion to monomers will be key – break even at ~0.4 g/L-hr + 50% conversion or ~0.5 g/L-hr + 40% conversion