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1.3.5.202

Hydrothermal Liquefaction Model Development

DOE Bioenergy Technologies Office (BETO)
2023 Project Peer Review
Advanced Algal Systems Program

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U.S. DEPARTMENT OF ENERGY BATTELLE

PNNL is operated by Battelle for the U.S. Department of Energy

Project Overview

Objective: Develop data-driven process models for techno-economic analysis (TEA) of algae hydrothermal liquefaction (HTL) processes to drive research and advance the state of technology (SOT).

Goals:

- Support the collaborative project: Hydrothermal Processing for Algal Based Biofuels and Co-products (1.3.4.101)
- Identify barriers and cost reduction strategies
- Assess sustainability impacts
- Inform technical and cost targets and track progress
- Document the SOT in annual assessments and case-study reports

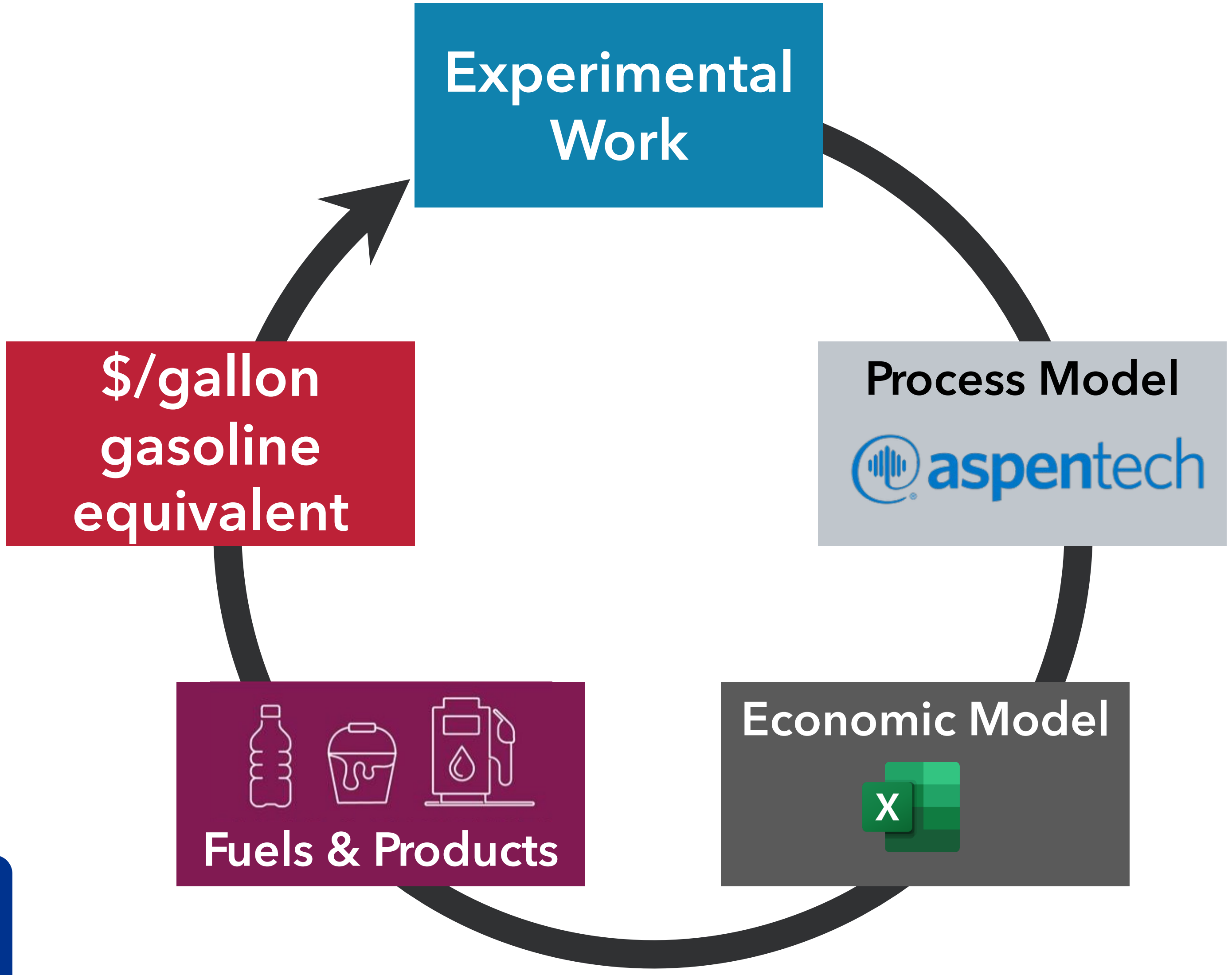
This project guides the experimental team to focus investigations on impactful cost-cutting measures and technology development.

Key Technical Developments:
System analysis for the conversion of algae via HTL is initiated.
Process model is updated to include algae/wood blends to supplement low-productivity seasons, reduce overall feedstock cost, eliminate algae drying expenses, and increase plant scale.
Sequential HTL processing is investigated to enable co-products and reduce overall costs.
Cost-advantaged algae feedstocks are modelled to improve process costs.
Production of sustainable aviation fuel is incorporated into the process and economic models.

1. Approach: Technical Objectives

- We work with the HTL researchers to **identify, interpret, and transform experimental results** to develop conceptual process and cost models to simulate commercial-scale plant performance and cost.
- We use models early in the research and development process to **identify and improve cost drivers**.
- We continually iterate with the experimentalist team to refine the technoeconomic model to reflect a **commercially relevant reality**.

Iteration of the technoeconomic modelling process enables data-driven decisions to maximize the impact of experimental work



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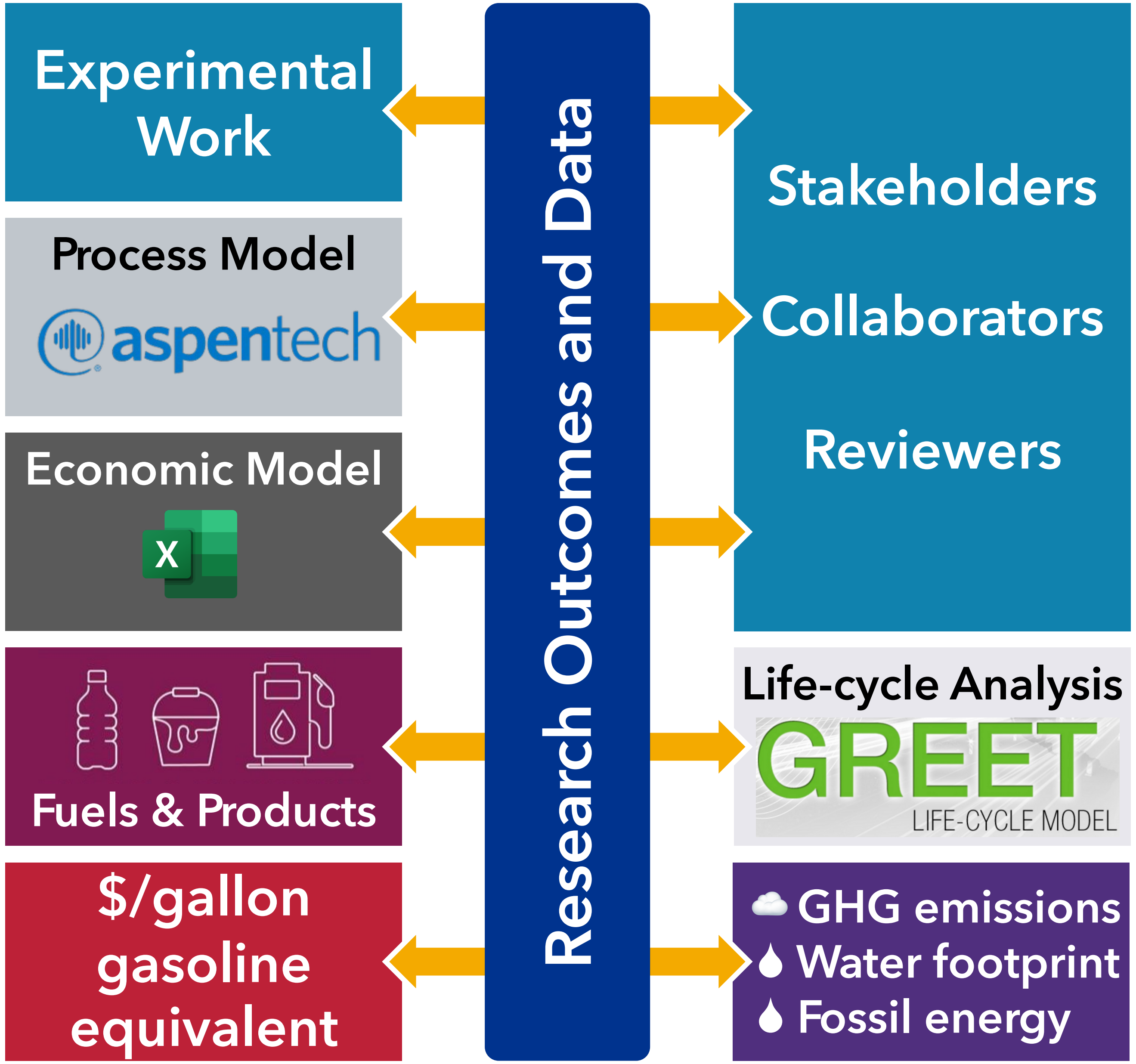
1. Approach: Technical Objectives

- We **engage with industrial collaborators** to understand processing and logistical challenges at scale, improve fidelity of our designs, and obtain realistic equipment costs to inform our models.
- We **provide life cycle inventory data** to Argonne National Laboratory for the life-cycle analysis and strategize on methods to reduce greenhouse gas (GHG) emissions.
- We **communicate technical results to the public** to promote interest in environmental sustainability and science, technology, engineering, and mathematics.

Engagement with external stakeholders, other national laboratories, and the public further enhances the value and impact of our work



1. Approach: Project Integration & Collaboration

The project is integrated with other project teams, national laboratories, and external collaborators to enable shared learning and to leverage a broad and diverse knowledge base

DISCOVR Consortium → Testing Material → **Algae Hydrothermal Processing PNNL & INL**

Algae Producers → Testing Material → **Algae Hydrothermal Processing PNNL & INL**

Algae Hydrothermal Processing
PNNL & INL

- Feedstock sourcing
- Algae HTL conversion
- Ash removal
- Co-product development

Hydrothermal Process Development Unit
PNNL

- HTL process scale-up (pumping, heat transfer, separations)
- Aqueous phase treatment
- Biocrude upgrading
- Industrial engagement

Experimental Data ↓ ↑ Cost Results

Shared learning through open inter-team communications

HTL Model Development
PNNL

- Techno-economic analysis
- Life-cycle inventory
- State-of-technology reports

NREL Algae Pond Model ↔ Cost Data ↔ **HTL Model Development PNNL**

ANL Sustainability ← Inventory Data ← **HTL Model Development PNNL**

ANL Sustainability → Life-cycle analysis → **HTL Model Development PNNL**

Bench Scale HTL of Wet Waste Feedstocks
PNNL

- Wet waste HTL conversion
- Feedstock analysis
- Biocrude upgrading
- Assessment driven research & development

1. Approach: Integration Across National Laboratories

Analysis projects supported by the Bioenergy Technologies Office

Analysis & Sustainability Interface @PNNL (Multi-criteria)
Strategic Analysis Support @NREL (Multi-criteria)
GREET Development @ANL (LCA)
Algae Lifecycle Analysis @ANL (LCA)

Supply Chain Strategic/Sustainability Analysis

Biomass Sourcing ▶ **Biomass Transport & Pre-processing Logistics** ▶ **Biorefinery Conversion** ▶ **End-Use Vehicle/Jet**

Biomass Sourcing

Supply Scenario Analysis @ORNL (Resource Assessment)

Microalgae Analysis @PNNL (Resource Assessment)

Algae System Techno-economic Analysis @NREL (TEA)

Biomass Transport & Pre-processing Logistics

Feedstock Supply Chain Analysis @INL (TEA)

Biorefinery Conversion

Biochemical Analysis @NREL (TEA)

Thermochemical Analysis @NREL (TEA)

Wet Waste HTL @PNNL (TEA)

Algae HTL @PNNL (TEA)

End-Use Vehicle/Jet

Feedstock Type
Terrestrial
Wet Waste
Algae

Argonne National Laboratory · Idaho National Laboratory · NREL National Renewable Energy Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory

1. Approach: Addressing Risk and Measuring Progress

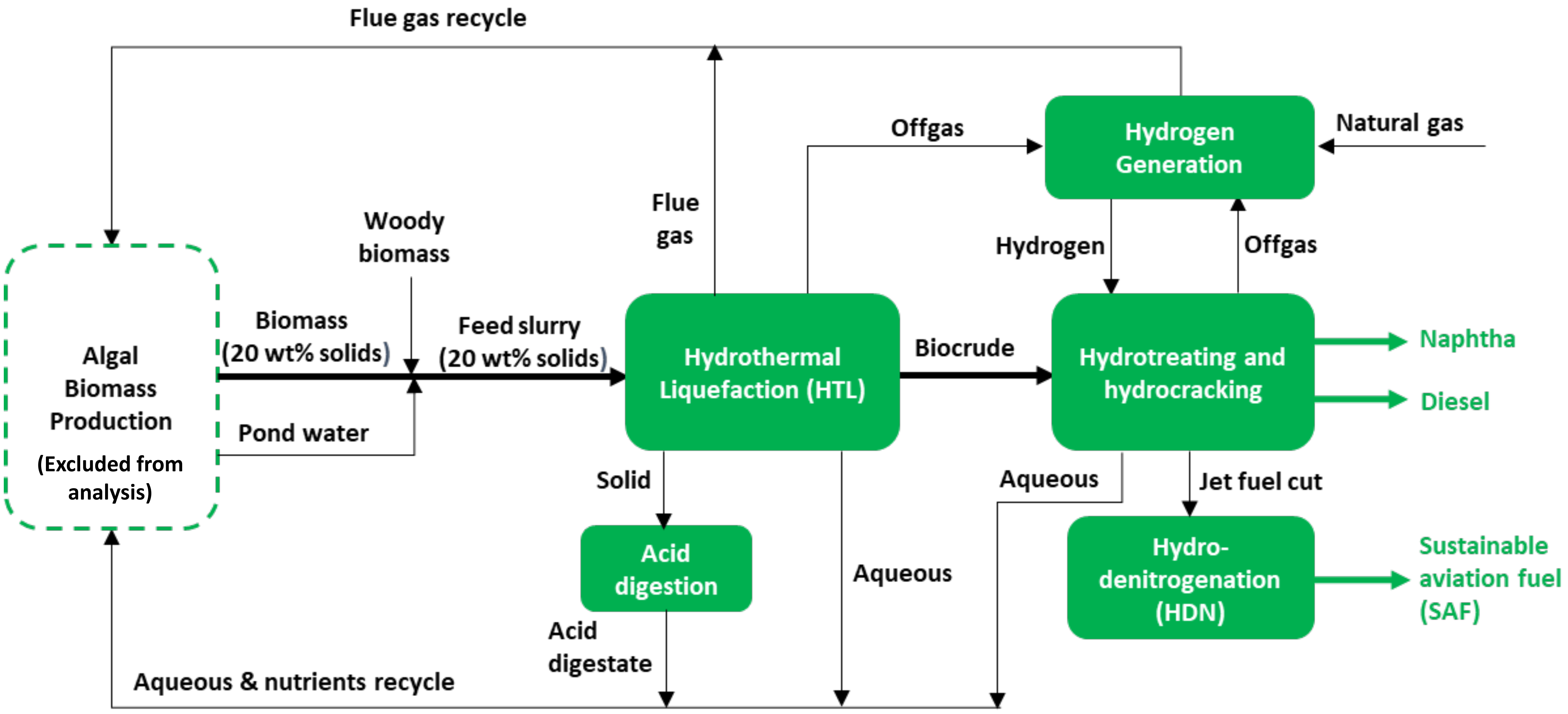
- Mitigation plans are ready to minimize technical and logistical risks to the project.
  - Mitigation plans allow for shift in approach to overcome potential challenges
  - Note: Risk mitigation plan is available in the supplemental slides

- Go/No-go decision at project midpoint (3/31/2023) measures progress against baseline for greenhouse gas (GHG) emissions from petroleum equivalents.

Go/No-Go Decision	Description	Criteria
Identify the combination of low-cost algae & co-product & HTL conversion that meets 2030 goals for GHG reductions	The research and development and supporting analysis conducted in fiscal years 2021 and 2022 will provide the basis of down-selection of low-cost algae feedstock strain, HTL process configuration (1- or 2-stage), and potential co-product to the most promising combination for near-term deployment and that can meet BETO's GHG reduction goals.	Deliver techno-economic and life cycle analysis report (supported with ANL analysis) for design that meets 70% GHG reduction targets.

1. Approach: Technical Objectives

Process boundary for the techno-economic model incorporates HTL, post-processing and recycle of by-products, and hydroprocessing and distillation of fuel products.



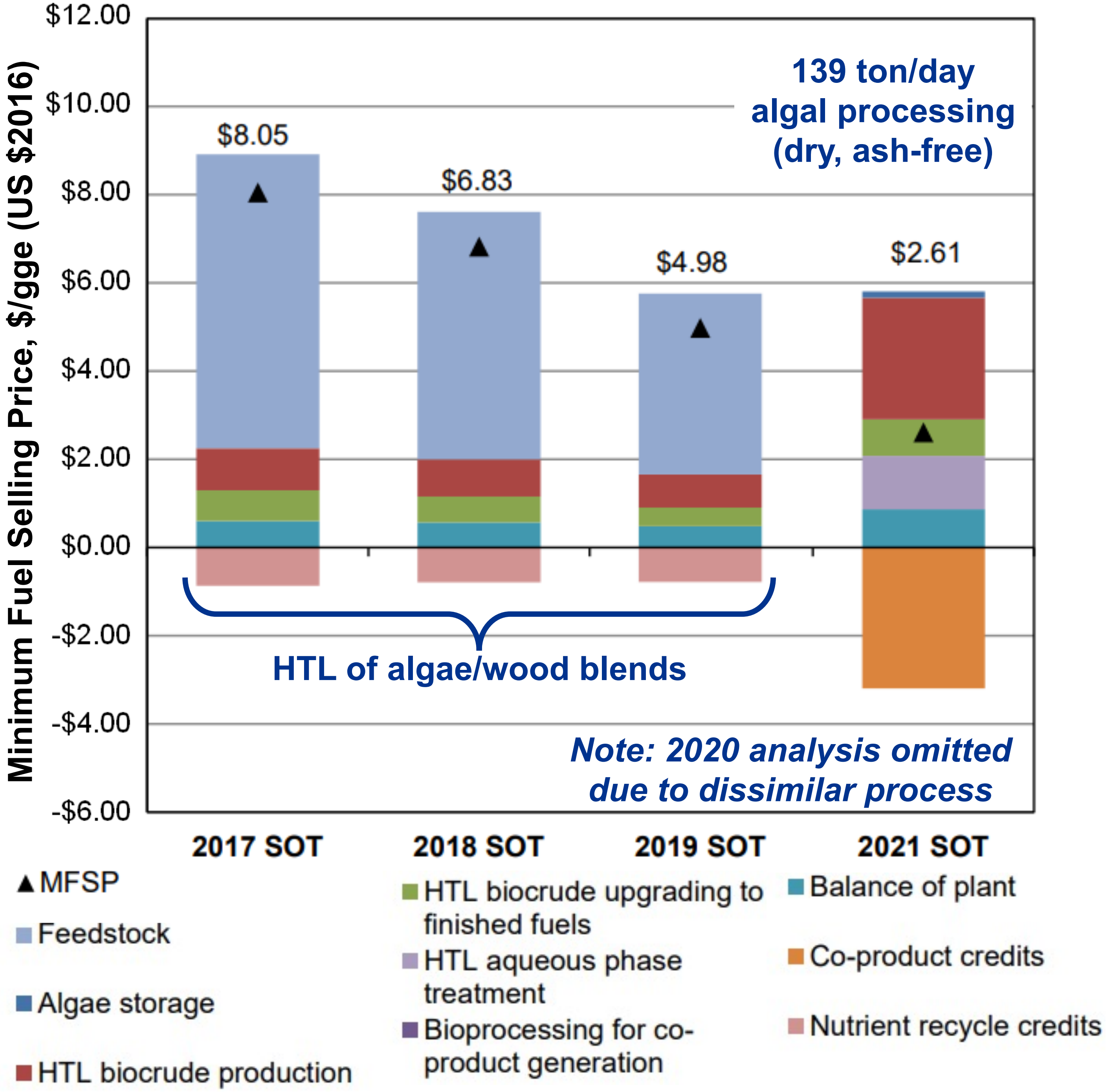
2. Progress and Milestones Since Last Peer Review

Hydrothermal conversion of cost-advantaged feedstock documented in 2021 SOT Report:

- Wastewater-grown algae enables reduced minimum fuel selling price **(MFSP) of $2.61/gge**
- **Greenhouse gas (GHG) emissions are reduced by 73%** compared to petroleum diesel (Cai et al. 2022, https://doi.org/10.2172/1862925)
- The sale of a co-product (struvite fertilizer) reduces net production costs and net GHG emissions (107% net reduction)

✓ Completed milestone on time: Delivery of 2021 State of Technology report

Significant progress towards economically and environmentally sustainable fuels



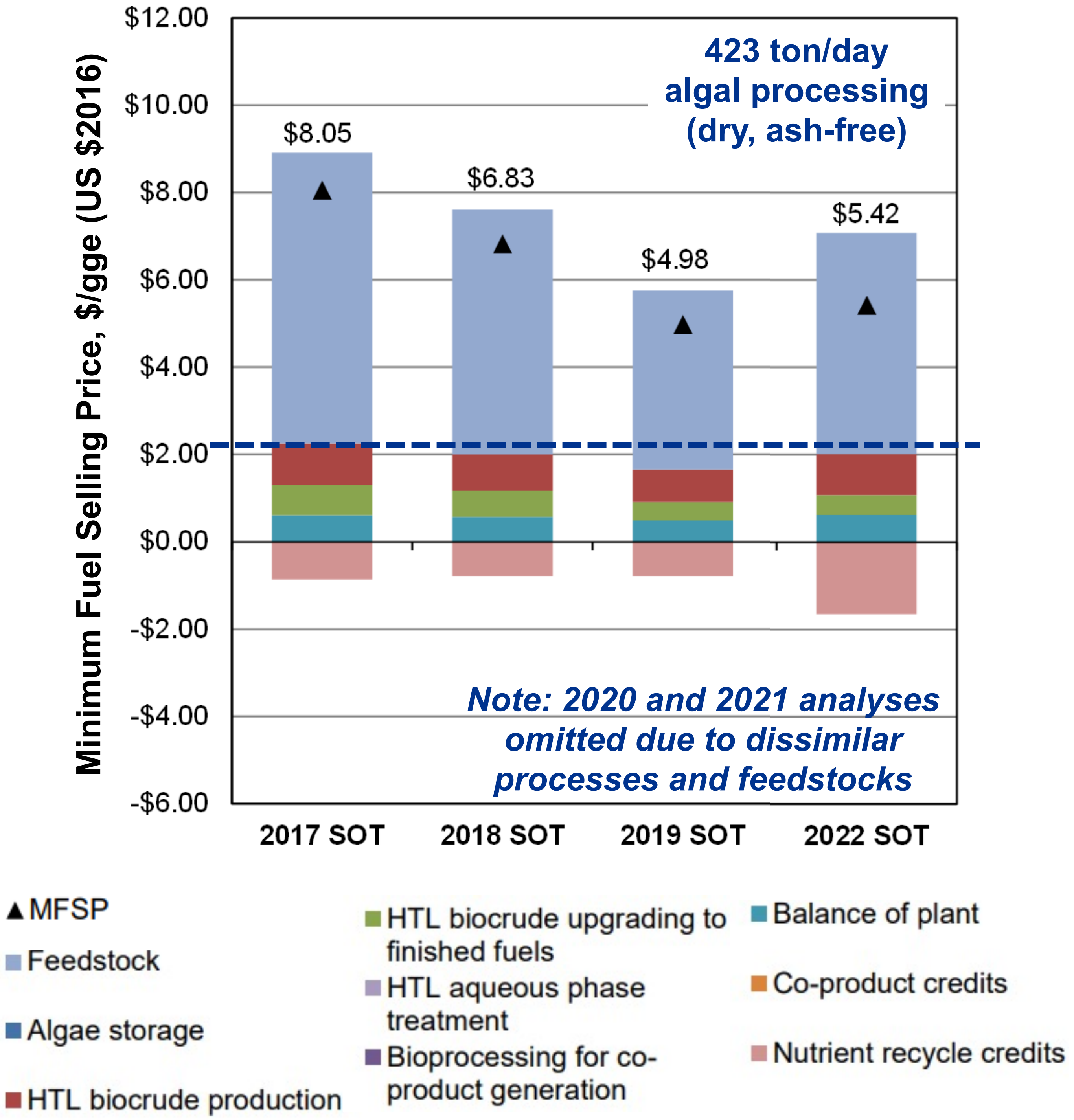
2. Progress and Milestones Since Last Peer Review

Hydrothermal conversion with production of sustainable aviation fuel (SAF) documented in 2022 SOT Report:

- Minimum fuel selling price (MFSP) is **$5.42/gge**
- Conversion costs are offset by the recycle of nutrients for algae cultivation
- Incorporation of denitrogenation step for SAF production contributes minimal cost (+$0.02/gge)

✓ Completed milestone on time: Delivery of draft version of 2022 State of Technology report

First report of an algae-to-SAF pathway via HTL



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2. Progress and Milestones Since Last Peer Review

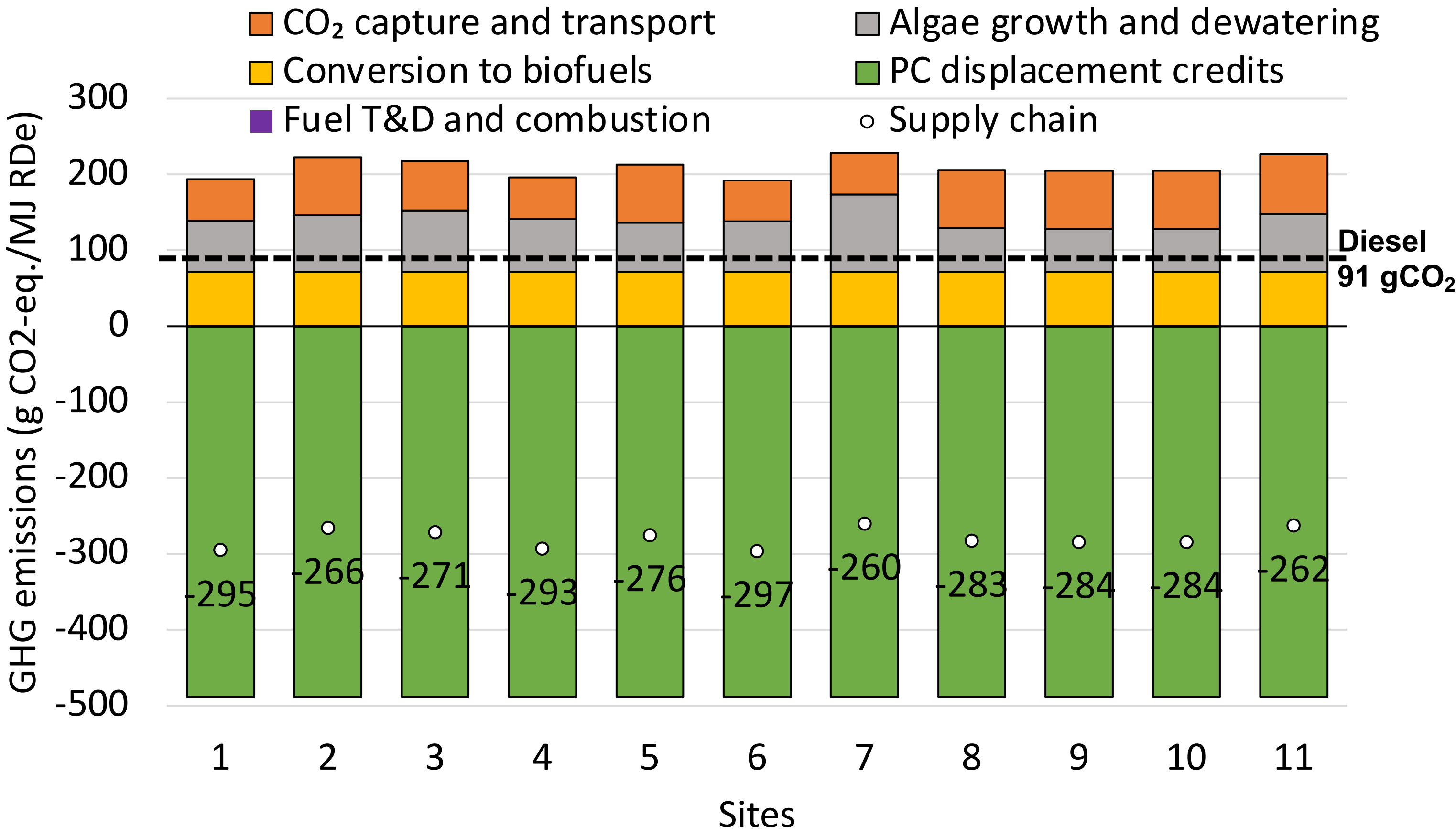
Support of the Algae Harmonization study:

- PNNL, NREL, and ANL collaborate to publish the Algae Harmonization study which documents near-term economic, sustainability, and resource potential for algal biomass opportunities.
- Upcoming version will include protein extracts and sustainable aviation fuels as products, investigating 11 geographic site groups.

	Baseline	Optimized
Algae processing (million metric tons per year)	162	162
Total fuel production (billion gallons per year)	27	9.3
Percent share of 2021 US gasoline consumption	20%	6.9%
Total protein concentrate production (million metric tons per year)	3.1	57
Weighted minimum fuel selling price ($ per gallon gasoline equivalent, gge)	$ 5.67	$ 3.51

In a cost-optimized scenario, with an unrestricted market for algal-derived proteins, the MFSP is $3.51/gge

Algal proteins generate displacement credits, resulting in net negative greenhouse gas (GHG) emissions



Draft results, not yet finalized

2. Progress and Milestones Since Last Peer Review

Support of research in the Development of Integrated Screening, Cultivar Optimization, and Verification Research (DISCOVR, 1.3.1.501) Consortium:

- Investigation of scenarios of single-strain nutrient replete/deplete pairs to determine the economic trade-offs between productivity and composition.
- TEA modeling investigation of a "crop rotation" strategy to represent a year-long cultivation cycle.

Collaboration across projects enables sharing of ideas and ensures consistent approaches in process modelling

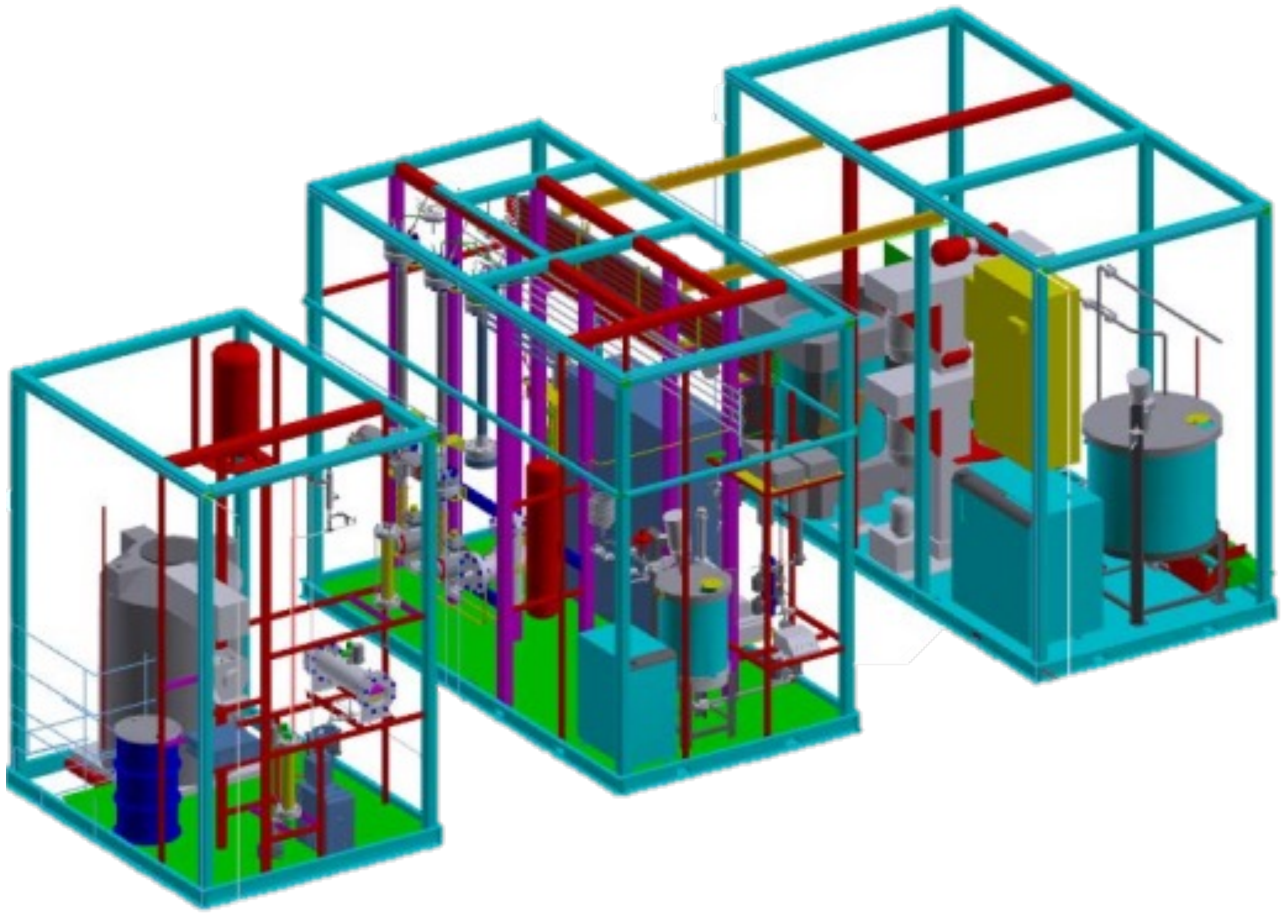
Lab-scale cultivation system of algae identified by the DISCOVR consortium

2. Current Project Progress

New Design Case Study reports will replace State of Technology reports to provide more design details to relevant stakeholders

Proposed Elements of a Design Case Study

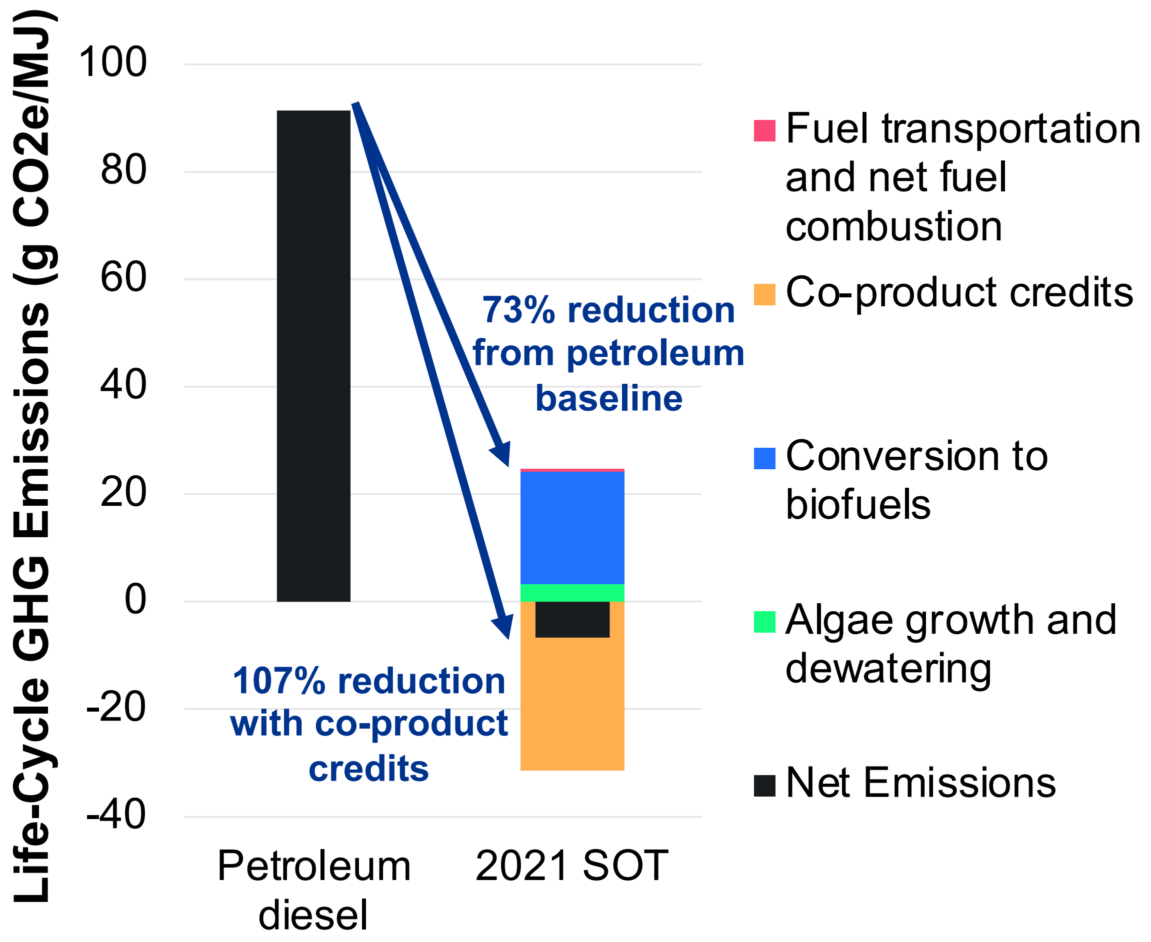
- Regional analysis of feedstock availability, scale, and costs
- Economics of a first-of-a-kind plant
- Technology readiness level assessment of major unit operations
- Sensitivity analysis of key variables
- A net-zero carbon case, utilizing renewable resources



3D model of the modular hydrothermal liquefaction system (MHTLS) at PNNL

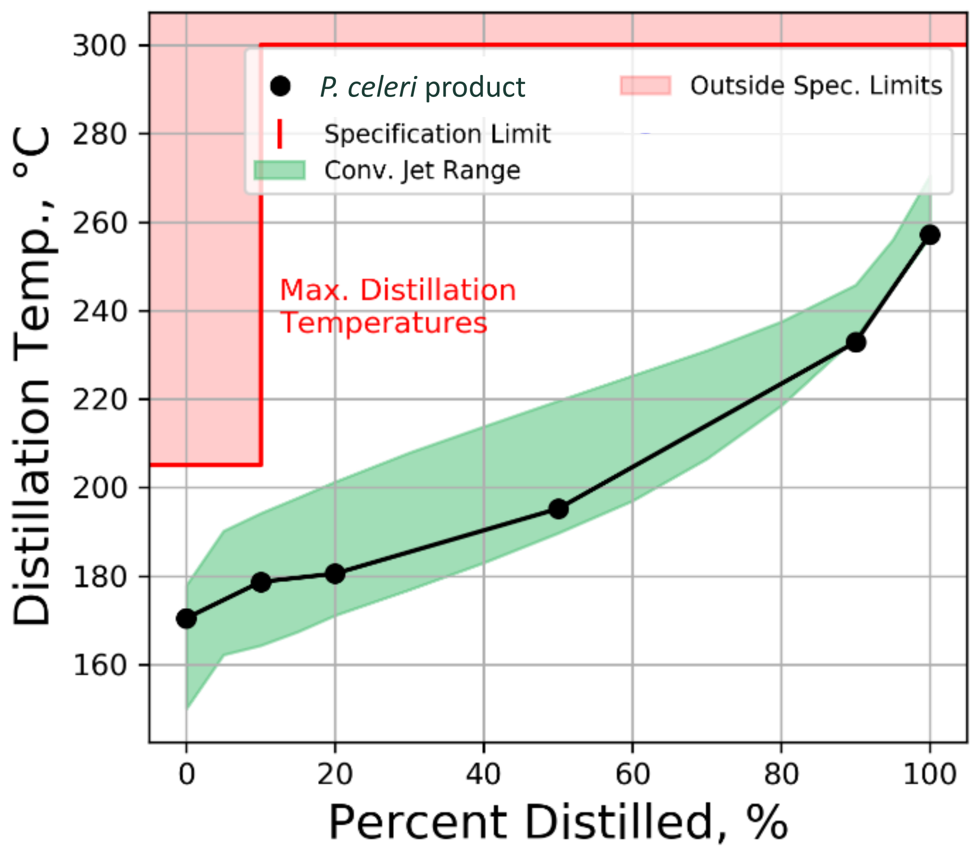
3. Impact: Technical and Commercial Significance

- Cost-advantaged feedstocks yields a favorable cost (**$2.61/gge**) and reduced GHG emissions (**73%**).



Data from Cai et al.(2022): doi.org/10.2172/1862925

- The production of SAF is possible from algae via HTL (**$5.42/gge**)
- 23% of upgraded biocrude is distilled within range of conventional jet fuel



Low-volume testing of algae-derived SAF meets specifications for jet fuel, additional results in supplemental slides

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3. Impact: Publicizing Results

- Since last peer review, the HTL Model Development project has released the 2021 and 2022 State of Technology reports

- Since inception, the Hydrothermal Liquefaction Model Development project has
  - provided content for or led **20 publications** and **20 presentations**
  - led to several **collaborative competitive projects** with DOE
  - led to several **industrial collaborations** and projects
  - supported the development of **several patents** and **licensing of technology** to industry.
  - Been awarded the **2015 FLC technology transfer excellence award** and the **2015 R&D 100 Award** “Hydrothermal Processing to Convert Wet Biomass into Biofuels”


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PNNL-32695

Hydrothermal Liquefaction and Upgrading of Wastewater-Grown Microalgae: 2021 State of Technology

March 2021

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PNNL-xxxxx

Microalgae Hydrothermal Liquefaction and Biocrude Upgrading: 2022 State of Technology

March 2023

Yunhua Zhu
Yiling Xu
Andrew Schmidt
Michael Thorson
Dylan Cronin
Daniel Santosa
Scott Edmundson
Shuyun Li
Lesley Snowden-Swan
Peter Valdez

U.S. DEPARTMENT OF ENERGY | Prepared for the U.S. Department of Energy under Contract DE-AC05-76RL01830

The project provides impact for DOE, the research community, and commercial partners

Summary

1 - Approach

- **Integrated project team** leveraging communications and expertise across project teams, national laboratories, and external collaborators
- Developed a project plan to address **data availability** and **technical risks**

2 - Progress

- Estimated the impact of using cost-advantaged algae, resulting in a minimum fuel selling price of **$2.61/gge** and a reduction of **GHG emissions by 73%**
- Estimated the cost of production of **sustainable aviation fuel** from *P. celeri* via HTL, resulting in a minimum fuel selling price of **$5.42/gge**

3 - Impact

- Demonstrated potential for cost-advantaged algae to produce **fuels and co-products at economically viable costs**
- Developed new **design case studies** to improve previous reporting methods
- Provided **continuous impact** from publications, presentations, awards, and collaborations

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Acknowledgements

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BETO Technology Manager

Phillip Lee
BETO Project Monitor

PNNL Project Team:

Yunhua Zhu
Yiling Xu
Shuyun Li
Peter Valdez
Lesley Snowden-Swan

National laboratory collaborators:

PNNL: Andre Coleman, Mark Wigmosta
NREL: Ryan Davis
ANL: Hao Cai
INL: Damon Hartley

Quad Chart Overview

Timeline
- Project start date: 10/01/2021
- Project end date: 9/30/2024

	FY 22	Total Award
DOE Funding	$200,000	$600,000 (negotiated total federal share over active project lifetime)

Related/Leveraged Projects
1.3.4.101 Hydrothermal Processing for Algal Based Biofuels and Co-products

1.3.2.501 Algae DISCOVR Project

2.2.2.301 PNNL Hydrothermal Process Development Units

TRL at Project Start: 3
TRL at Project End: 4

Project Goal
Employ TEA coupled with researcher input and feedback to guide and track research towards reducing the costs of renewable fuels and co-products from biomass via HTL; HTL biocrude upgrading to fuels and HTL aqueous carbon recovery and utilization.

End of Project Milestone
Complete 2024 SOT assessment and report draft, showing progress toward 2030 $2.5/GGE target and 70% greenhouse gas emissions reduction. Submit life-cycle inventory to Argonne National Laboratory for sustainability analysis

Funding Mechanism
2023 Lab Call

Project Partners
- ANL: Life cycle analysis
- INL: Terrestrial feedstock cost and quality
- NREL: Algal feedstock cost and availability
- PNNL: Experimental teams and resource analysis

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Thank you

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Supplemental Information

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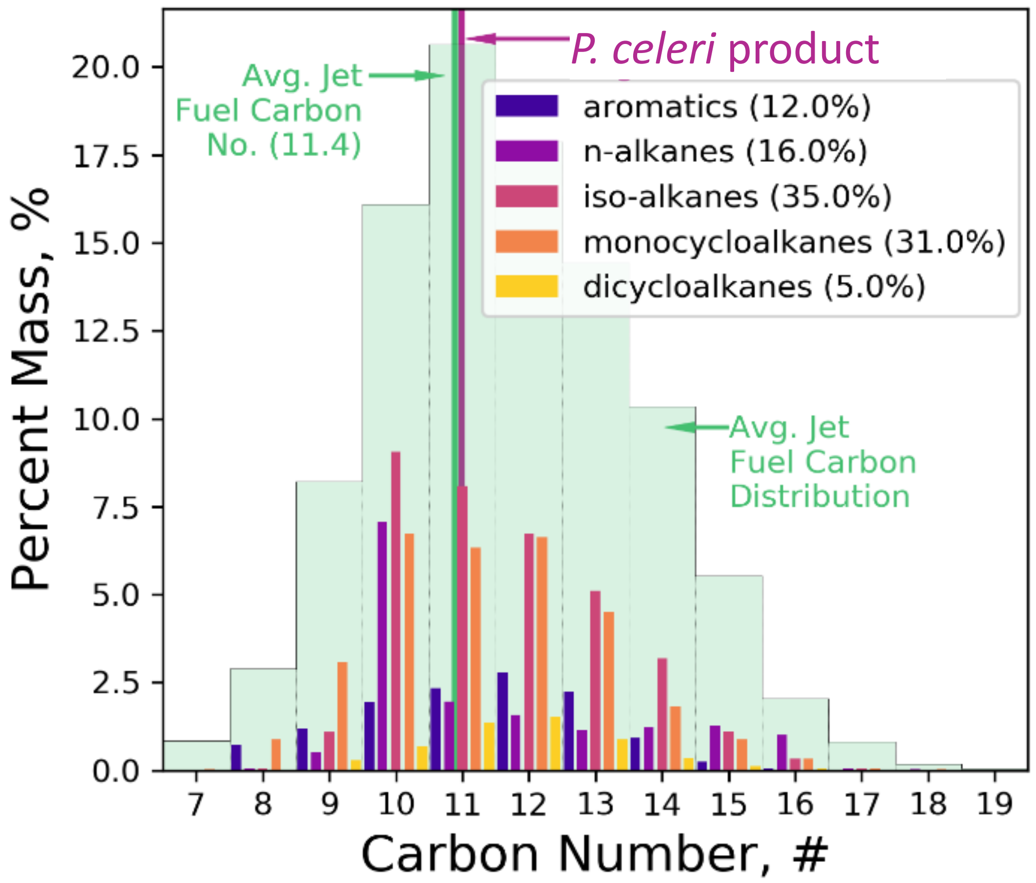
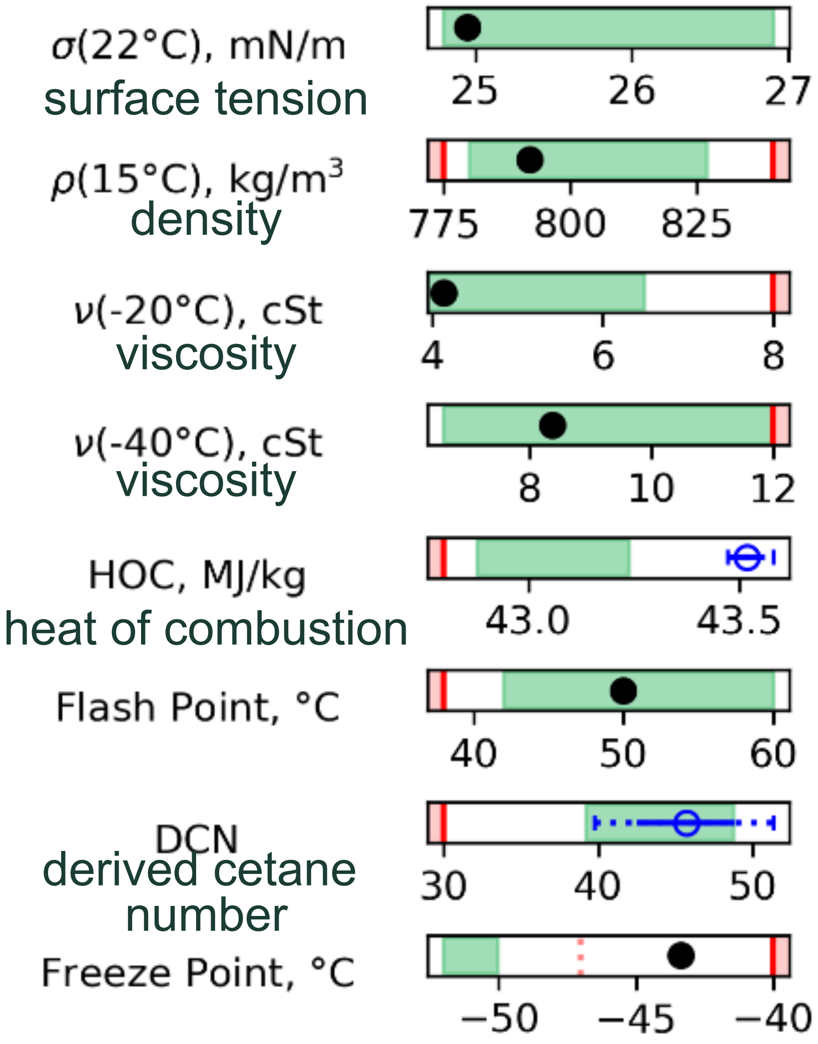
Risk Mitigation Plan

Project Risks	Mitigation Plan
Lack of data availability to complete the SOT on time. Uncertainty in the choice of conversion pathways for the SOT and design case.	Mitigate by scheduling regular meetings with researchers and continuous feedback and communication with BETO.
A common basis is needed across labs for assumptions and parameters for TEA/LCA to ensure consistent pathway evaluation and comparisons.	Mitigate by timely discussions with BETO, NREL, and ANL and carry out joint Lab harmonization study.

Additional results for assessment of upgraded and distilled biocrude from *P. celeri*



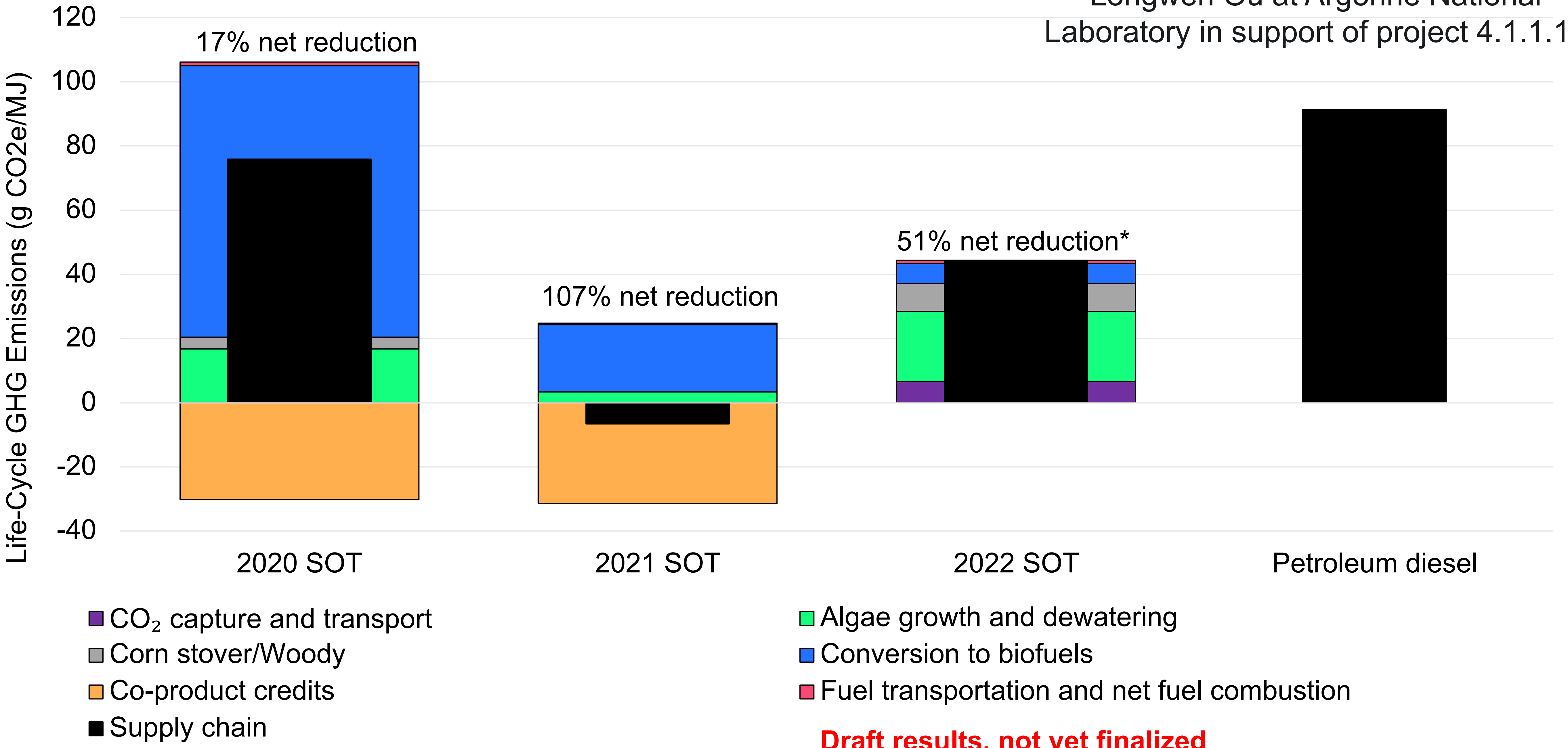


Low-volume testing of algae-derived SAF meets specifications for conventional jet fuel

- Measured value
- Predicted value and range
- Specification limit
- Outside of specification range
- Conventional range for jet fuel

Greenhouse gas emissions for algae hydrothermal liquefaction scenarios

Results generated by Hao Cai and Longwen Ou at Argonne National Laboratory in support of project 4.1.1.10



Draft results, not yet finalized

Responses to Previous Reviewers' Comments

FY21 Peer Review Report for Advanced Algal Systems *https://www.energy.gov/sites/default/files/2022-06/beto-02-Advanced-Algal-Systems-2021-peer-review.pdf*

Comment 1: *"The claim of "780 dry tons/day based on POND model = 6,800x scale increase from data" is a tremendous leap, and even small errors in assumptions could constitute large risks to ultimate project success. This model's greatest source of weakness is likely not uncertainty about offtake markets, but lack of information about costs for maintenance and operations."*

Response 1: The plant scale assumed is consistent with BETO's algae pond model scale. We agree that larger-scale field testing of algae production is ultimately needed to reduce uncertainties around the performance assumptions and TEA at a commercial scale. Regarding the conversion process, we expect to use our engineering scale HTL system (12x larger than bench) for sequential HTL testing in the future, which should provide insight closer to real-world operation and help identify scale-up issues. Our design case and SOT reports include detailed process design information and are made available to the public on the DOE Office of Scientific and Technical Information website. The primary purpose of our analyses is to determine feasibility early in the concept stage and guide and track progress in BETO's R&D toward reducing costs and improving the viability of the technology. A rigorous engineering design estimate by an engineering, procurement, and construction firm would be needed to support decision-making around actual project construction.

Comment 2: *"A model that can predict HTL outputs based on easily translated feedstock composition metrics would be the most impactful work this team could do to make this technology approachable for potential users."*

Response 2: We agree that being able to systematically correlate incoming feedstock composition with biocrude and fuel properties is of great value. To this end, we have developed reduced-order models based on PNNL's extensive library of continuous testing data to predict yield and quality for both algae- and waste-derived biocrudes from single-stage HTL (https://doi.org/10.1016/j.algal.2019.101450; https://doi.org/10.1016/j.apenergy.2020.116340). Our SEQHTL work is relatively new, but as more testing data sets are generated, a predictive model can be developed in the future.

Comment 3: *"The team has done a great job in working with researchers and industrial partners to ensure that assumptions used in the model reflect real-life processes. However, the team should consider upgrading the cost of coproducts to reflect actual costs based on the different processes as opposed to a fixed cost for coproducts."*

Response 3: Regarding costing of the coproducts, the analysis estimates the minimum fuel selling price using a fixed coproduct market price, consistent with the other BETO pathway analyses. Another perspective, as the reviewer points out, is to calculate the minimum coproduct selling price using a fixed fuel selling price. We appreciate the comment made by the reviewer and will work to include it in future analysis.

Publications, Patents, Presentations, Awards, and Commercialization since 2021 Peer Review

Publications

20. Zhu, Y., Y. Xu, A. Schmidt, M. Thorson, D. Cronin, D. Santosa, S. Edmundson, S. Li, L. Snowden-Swan, P. Valdez. (2022). "Microalgae hydrothermal liquefaction and biocrude upgrading: 2022 State of Technology." PNNL-XXXXX. In Progress.

19. Santosa D.M., L. Wendt, B.D. Wahlen, A.J. Schmidt, J.M. Billing, I.V. Kutnyakov, and R.T. Hallen, et al. 2022. "Impact of Storage and Blending of Algae and Forest Product Residue on Fuel Blendstock Production." *Algal Research* 62 (2022) 102622. https://doi.org/10.1016/j.algal.2021.102622

18. Zhu, Y., A. J. Schmidt, P. J. Valdez, L. J. Snowden-Swan and S. J. Edmundson (2022). Hydrothermal Liquefaction and Upgrading of Wastewater-Grown Microalgae: 2021 State of Technology. PNNL-32695. https://doi.org/10.2172/1855835

17. Zhu, Y., S. B. Jones, A. J. Schmidt, H. M. Job, J. M. Billing, J. R. Collett, K. R. Pomraning, S. P. Fox, T. R. Hart, S. J. Edmundson, M. R. Thorson, P. A. Meyer, L. J. Snowden-Swan and D. B. Anderson (2021). "Microalgae Conversion to Biofuels and Biochemical via Sequential Hydrothermal Liquefaction (SEQHTL) and Bioprocessing: 2020 State of Technology." PNNL-30124. https://doi.org/10.2172/1784347

Presentations

20. Valdez, P., A. Schmidt, S. Edmundson, T. Hart, D. Cronin, S. Fox. 2022. "Overcoming Engineering Challenges for the Hydrothermal Liquefaction of Cost-Advantaged Algal Feedstocks". AIChE Annual Meeting, Phoenix, AZ.

19. Zhu Y., S.B. Jones, A.J. Schmidt, J.M. Billing, J.R. Collett, L.J. Snowden-Swan, and D.B. Anderson. 2021. "Preliminary Economic Analysis of Microalgae Conversion to Biofuels and Biochemical via Sequential Hydrothermal Liquefaction (SEQHTL) and Bioprocessing." The International Conference on Algal Biomass, Biofuels and Bioproducts 2021, Online Conference.

Past Patents, Awards, and Commercialization Activities

Awards

- 2015 FLC technology transfer excellence award
- 2015 R&D 100 Award “Hydrothermal Processing to Convert Wet Biomass into Biofuels”

Patents and Patent Applications

- Mike Thorson, Lesley Snowden-Swan, Andy Schmidt, Todd Hart, Justin Billing, Dan Anderson and Rich Hallen. Filed January 2020. “Hydrothermal liquefaction system” U.S. Patent #11,279,882.
- Mike Thorson, Rich Hallen, Justin Billing, Andy Schmidt, Todd Hart, and Teresa Lemmon. Filed December 2019. “MOVING BED PRETREATMENT FOR IRON-CONTAINING BIOCRUDE.” US Pat Appl 31594/ 9760.
- Elliott, D.C.; Oyler, J.R. Issued on November 4, 2014. "Methods for Sulfate Removal in Liquid-Phase Catalytic Hydrothermal Gasification of Biomass." U.S. Patent #8,877,098.

Previous Publications

16. Zhu Y, SB Jones, AJ Schmidt, JM Billing, MR Thorson, DM Santosa, RT Hallen, and DB Anderson. 2020. "Algae/Wood Blends Hydrothermal Liquefaction and Upgrading: 2019 State of Technology." PNNL-29861. https://doi.org/10.2172/1616287
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10. Jessica Tryner, Karl Albrecht, Justin Billing, Richard T. Hallen, and Anthony J. Marchese. 2017. "Performance of a Compression Ignition Engine Fueled with Renewable Diesel Blends Produced from Hydrothermal Liquefaction, Fast Pyrolysis, and Conversion of Ethanol to Diesel."
9. Edmundson S.J., M. Huesemann, R. Kruk, A. Schmidt, T. Lemmon, J. Billing, and D. Anderson. "Phosphorus and Nitrogen Recycle Following Algal Bio-crude Production via Continuous Hydrothermal Liquefaction." *Algal Research*, 26, 415-421. https://doi.org/10.1016/j.algal.2017.07.016

Previous Publications

8. Jacqueline M Jarvis; Justin M Billing; Yuri E Corilo; Andrew J Schmidt; Richard T Hallen; Tanner Schaub, Ph.D. “FT-ICR MS analysis of blended pine-microalgae feedstock HTL biocrudes.” *Fuel* 216, 341-348. https://doi.org/10.1016/j.fuel.2017.12.016
7. Jarvis JM, N Sudasinghe, KO Albrecht, AJ Schmidt, RT Hallen, DB Anderson, JM Billing, and T Schaub. 2016. "Impact of Iron Porphyrin Complexes when Hydroprocessing Algal HTL Biocrude." *Fuel* 182:411-418. https://doi.org/10.1016/j.fuel.2016.05.107
6. He Y, X Li, X Xue, MS Swita, AJ Schmidt, and B Yang. 2017. "Biological Conversion of the Aqueous Wastes from Hydrothermal Liquefaction of Algae and Pine Wood by Rhodococci." *Bioresource Technology* 224:457-464. https://doi.org/10.1016/j.biortech.2016.10.059
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2. Maddi, B.; Panisko, E.; Wietsma, T.; Lemmon, T.; Swita, M.; Albrecht, K.; Howe, D. 2016. “Quantitative characterization of the aqueous fraction from hydrothermal liquefaction of algae.” *Biomass and Bioenergy*, 93, 122-130. https://doi.org/10.1016/j.biombioe.2016.07.010
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Previous Presentations

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