DOE Bioenergy Technologies Office (BETO) 2023 Project Peer Review

Thermochemical Platform Analysis

WBS: 2.1.0.302

April 6, 2023
Catalytic Upgrading
Abhijit Dutta (PI)
NREL

Key Contributors: Abhijit Dutta, Michael Talmadge, Kylee Harris, Geetanjali Yadav

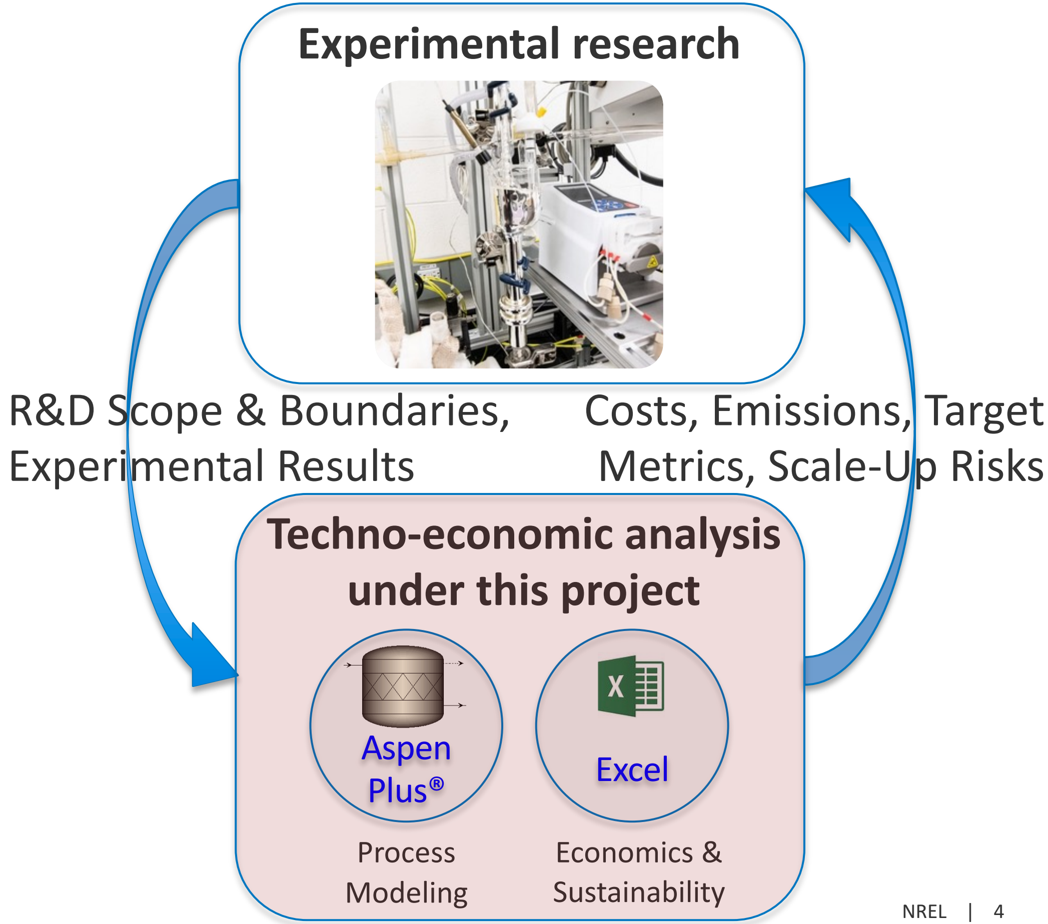
Acronyms Used

BETO: Bioenergy Technologies Office
CCPC: Consortium for Computational Physics and Chemistry
CFP: Catalytic Fast Pyrolysis
DEI: Diversity Equity Inclusion
DME: Di-Methyl Ether
FCC: Fluid Catalytic Cracking
FCIC: Feedstock-Conversion Interface Consortium
FP: Fast Pyrolysis
FY: Fiscal Year (e.g., FY23 is fiscal year 2023)
GGE: Gallon Gasoline Equivalent
HOG: High-Octane Gasoline
HT: Hydrotreating
LCA: Life-Cycle Analysis
MFSP: Minimum Fuel Selling Price
MYP: Multi-Year Plan (BETO)
SAF: Sustainable Aviation Fuel
SCSA: Supply Chain Sustainability Analysis
SOT: State of Technology
STH: Syngas to Hydrocarbons
TEA: Techno-Economic Analysis

Project Overview

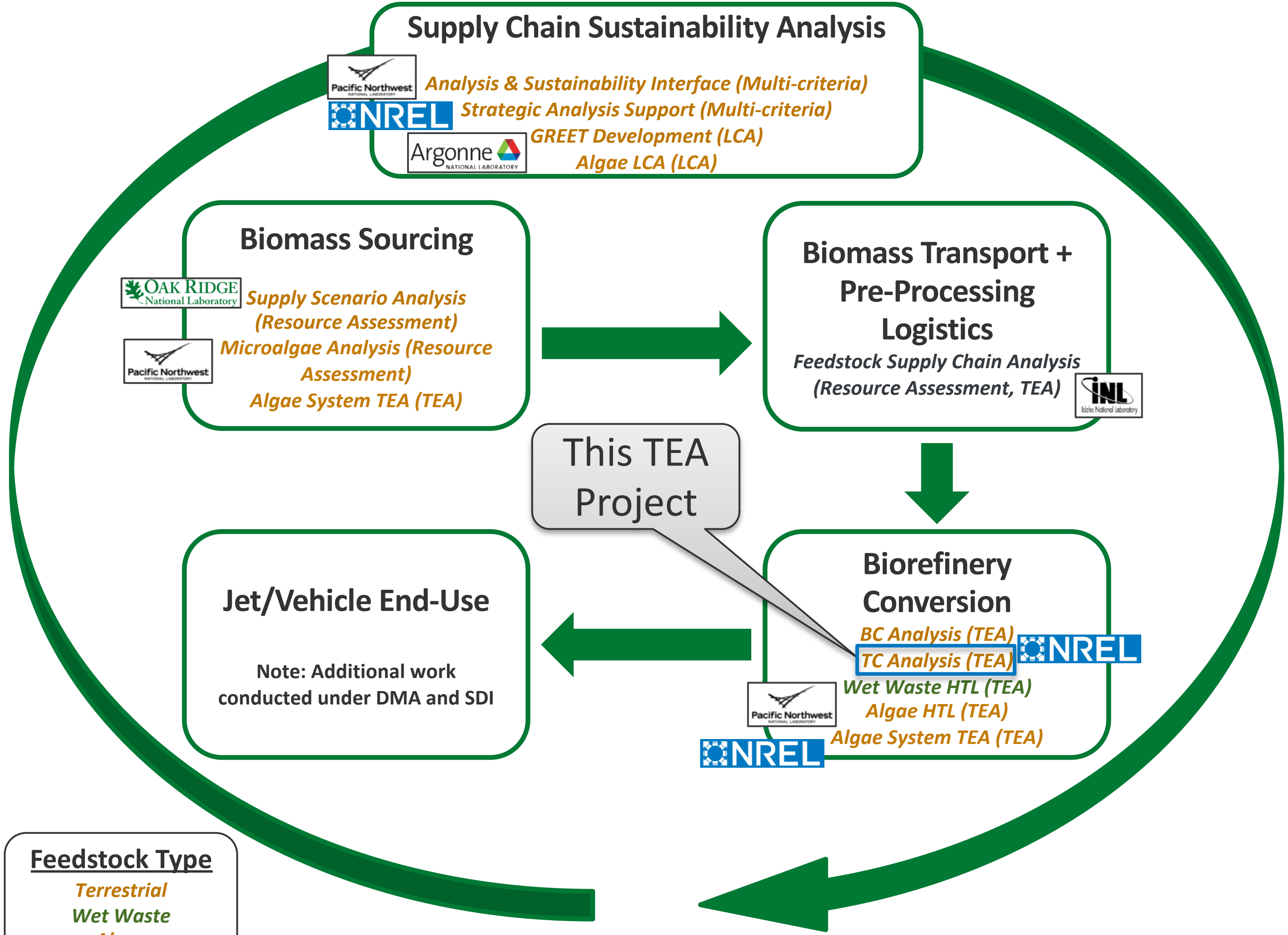
Overview

- Primarily focused on **techno-economic analysis (TEA)** and **process sustainability**
- Helps **guide research** in productive directions
  - *No direct experimental research under this project*
- Provides **industrial context and risk information** for research activities



Overview

BETO Analysis Projects Portfolio



SCSA: Supply Chain Sustainability Analysis
TEA: Techno-Economic Analysis
DMA: Data Modeling and Analysis
SDI: Systems Development and Integration

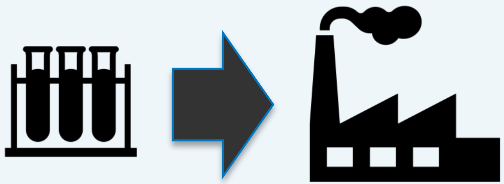
Feedstock Type

Terrestrial
Wet Waste
Algae

Overview

Overview of Project Goals

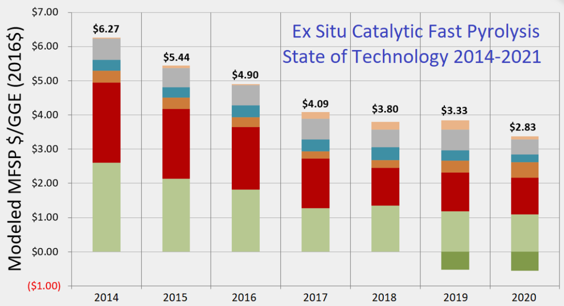
Improve Research Impacts by Providing Industrial Context



Lab R&D relevant for future scale-up?

Previous Focus

Annual State of Technology (SOT) Assessments towards Modeled Cost Targets



Help Identify Risks & Fill Gaps

Mitigate scale-up risks feasible within lab/pilot research. Enable stakeholders

Maximize SAF and Heavy Fuels as Primary Products

SAF: Sustainable Aviation Fuel

Facilitate the Reuse of Existing Petroleum Refining Operations

Help achieve BETO's goals towards SAF & liquid fuels for pyrolytic & syngas conversion pathways

Approach

Approach

Support Core Thermo-Catalytic Research Projects

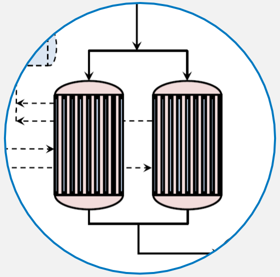
Core Research Areas

Thermo-Catalytic Conversion

Pyrolytic Biocrudes

WBS 2.3.1.314

Catalytic Upgrading of Pyrolysis Products for Production of SAF



Syngas Conversion

WBS 2.3.1.305

Upgrading of C1 Building Blocks

Current Focus

Refinery Processing & Fuel Compatibility

- Co-hydrotreating
- Standalone hydrotreating
- Assess other relevant refinery operations
- Vet assumptions

Synthetic Liquid Fuels

- Direct C_{4+} hydrocarbons from syngas
- Next step: C_{4+} to jet
- Waste & CO_2 use

Industrial Feedback and Risk Mitigation

Support & Collaboration

Catalyst R&D, Experimental Data

Collaboration with

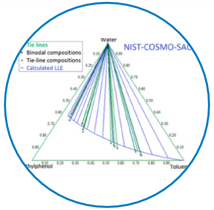
ChemCatBio
Chemical Catalysis for Bioenergy

Feedstock

Collaboration with

INL Idaho National Laboratory

fcic



Fuel Property Predictions

Collaboration with

NIST

Some other collaborations:

Johnson Matthey

Pacific Northwest NATIONAL LABORATORY

Consortium for Computational Physics and Chemistry

Argonne NATIONAL LABORATORY

Technical Approach for Analysis Work

Level of Detail Based on Requirement & Research Stage

Tools Used and Other Inputs

- Aspen Plus® — **Process Model**
- Excel — **Economics**
- GREET LIFE-CYCLE MODEL, ANL — **Life-Cycle Analysis**

- **Research Data:** Experiments, researchers, and literature
- **Capital & Operating Costs:** Literature, vendor quotes, Aspen Capital Cost Estimator
- **Financial and Feedstock Assumptions:** Consistent with BETO guidelines & related feedstock research

Outputs

- **MFSP (Minimum Fuel Selling Price)** based on nth plant economics & financial assumptions
  - SOT (State of Technology)
  - Projections
- **Technical metrics** to achieve MFSP
- **Sustainability metrics** of the conversion process
- Full LCA by ANL
- Review comments and **feedback from stakeholders are incorporated**

LCA: Life-Cycle Assessment, **ANL:** Argonne National Laboratory

Approach

Collaborators and Communication

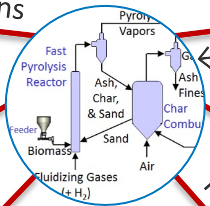
Results from Experiments

NREL, PNNL & Others

External Expert Reviews: Comments Addressed & Communicated Back

Core TEA

Annual Operating Plan



Outputs for Stakeholders: Reports, Publications, Models

Sustainability Analysis

Argonne National Lab

← Technical targets & Research Options

Experimental Results →

Process Lifecycle Inventory →

← Lifecycle Analysis for Entire Process, Including Feedstock Impact

← Model Specifications

Equipment Cost →

← Modeling Needs

Compatible Custom Model →

System of Compounds →

Predictive Models

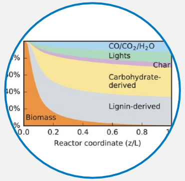
← Feedstock Cost & Associated Specifications

Feedstock Constraints →

Custom Cost Estimates

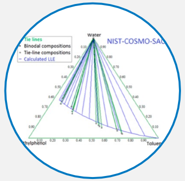
Subcontracts & Vendors

Custom Models



CCPC & Subcontracts

Product Properties



NIST & Subcontracts

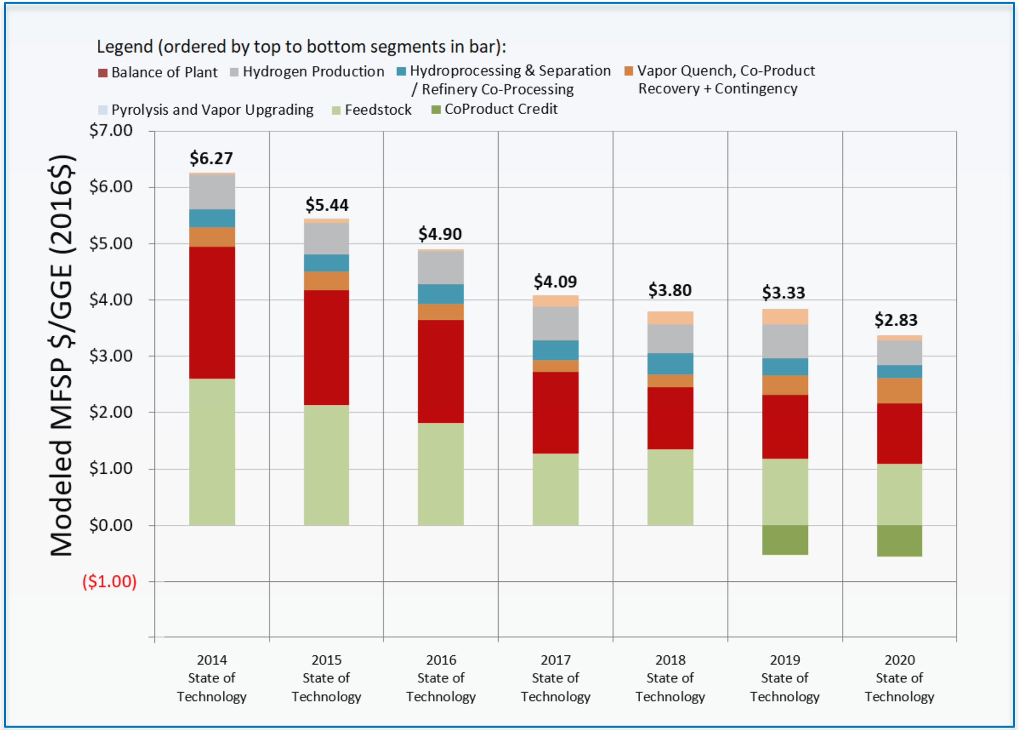
Feedstock Specs & Cost

Idaho National Lab & FCIC

NIST: National Institute of Standards and Technology. **CCPC:** Consortium for Computational Physics and Chemistry. **FCIC:** Feedstock-Conversion Interface Consortium. **TEA:** Techno-Economic Analysis

Change in Focus: Emphasis on Industrial Impact & SAF

Previous Approach: Focus on annual SOT (State of Technology) reports with modeled cost reduction



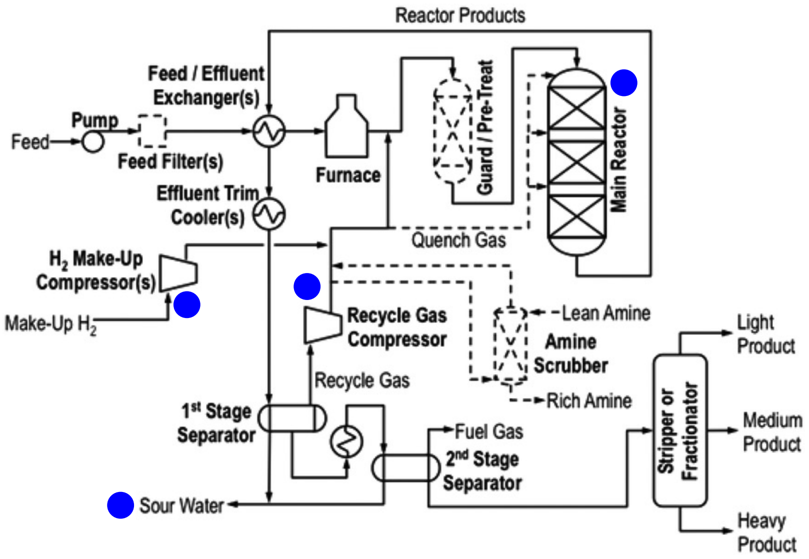
CFP: Catalytic Fast Pyrolysis; **SOT:** State of Technology;
MFSP: Minimum Fuel Selling Price; **SAF:** Sustainable Aviation Fuel

New Approach (focus):

- *Tighter integration of TEA & LCA*
  - Help decarbonization goals
  - Identify low emission options
- Prominence of *scale-up and risk assessments* for industrial implementations & relevance
  - Broaden sensitivity analysis
  - Advance refinery processing
- Enable research success and process scale-up for syngas to SAF
- Address constraints for SAF production & quality. *Leverage beneficial properties*:
  - Cycloalkanes from CFP
  - Iso-alkanes from syngas

Refinery Integration Analysis for Pyrolytic Biocrudes

Standalone models available.
Build detailed coprocessing models



Some hydroprocessing impact areas

Integration cost assessments

- Identify bottlenecks introduced to refinery operations based on Aspen Plus® model results
- Develop debottlenecking costs
  - Work with **KBR**

Effective use of experimental results

- Use experimental results to inform technical feasibility & model inputs
- Feedback loop with experimental work to identify risks and inform mitigation strategies
- Include fuel quality in models
  - Assess SAF compatibility, overall costs & GHG emissions
- *Build model options: focus on configurations meeting SAF quality*

Figures from: Talmadge et al., Green Chem., 2014,16, 407-453.

Approach

Expert Feedback for Relevance & Risk Identification

Reports & Model Assumptions Reviewed

Technology experts for relevance/risk identification

- Engineering firm/consultants during design
- Advisors for expert reviews and feedback

Example of relevant expert consultation/feedback

2015 Design Report

NREL NATIONAL RENEWABLE ENERGY LABORATORY

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle *Since 1965*

Technical Report
NREL/TP-5100-62455
PNNL-23823
March 2015

Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels

Thermochemical Research Pathways with *In Situ* and *Ex Situ* Upgrading of Fast Pyrolysis Vapors

Harris Group Inc.

DWH Process Consulting

Consultants

Expert Reviewers

National Renewable Energy Laboratory	Bob Baldwin, Mary Biddy, Danny Carpenter, Mark Davis, Kristiina Iisa, Calvin Mukarakate, Joshua Schaidle, Stefan Czernik (retired)
Pacific Northwest National Laboratory	Doug Elliott, Sue Jones, Mariefel Olarte, Alan Zacher
Idaho National Laboratory	Jake Jacobson
Argonne National Laboratory	Felix Adom, Jennifer Dunn
BP	Peter Metelski
Colorado School of Mines	Robert Braun
Cool Planet Energy Systems	Daren Daugaard
ExxonMobil Chemical Company	Gerry McGlamery
Global Energy Management Institute (University of Houston) and AOTA Energy Consultants	Steve Arbogast, Dave Paynter, Jim Wykowski
Iowa State University	Mark Wright
Johnson Matthey	Raymond Hadden, Andrew Heavers, Mike Watson
Pall Corporation	Mark Hurwitz
RTI International	David Dayton
University of Maine	William DeSisto
VTT Technical Research Centre of Finland	Yrjo Solantausta, Kristin Onarheim

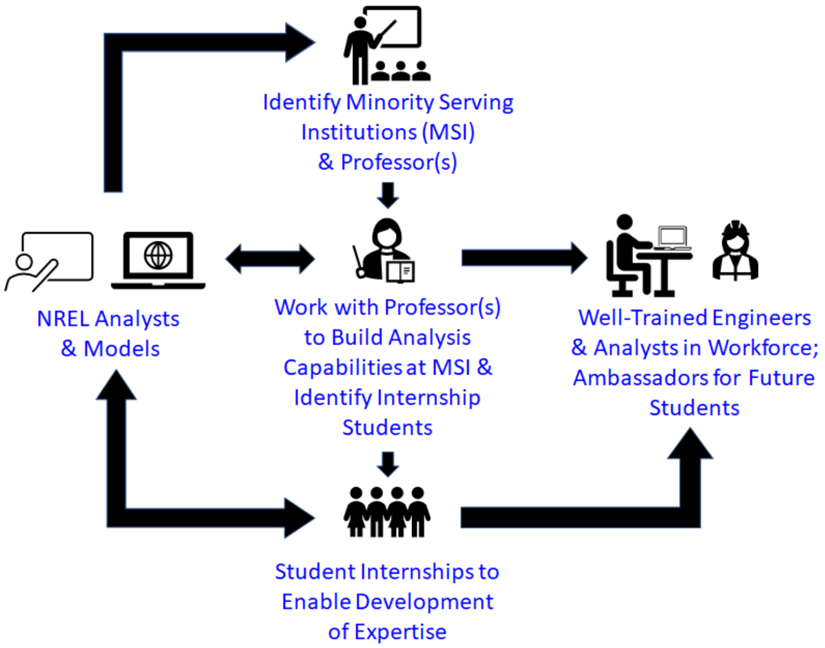
Transparency of comments & responses

Appendix J. Reviewer Comments on Draft Design Report and Responses

This appendix presents a summary of reviewer comments from draft versions of the report, issued for peer review in June 2014 and in August 2014. Comments from the peer review panel are summarized below and followed by a response from the authors. Some of the comments are paraphrased along with added context for clarity. Comments were combined when there were commonalities among observations from multiple reviewers. Minor/editorial comments were addressed, but left out of this appendix. The responses also describe any actions taken to address the comments in this final version.

Diversity Equity Inclusion (DEI) Plan

Plan to work with identified Minority Serving Institution(s) to help build their bioconversion TEA capabilities during this project cycle (FY 2023 to 2025)



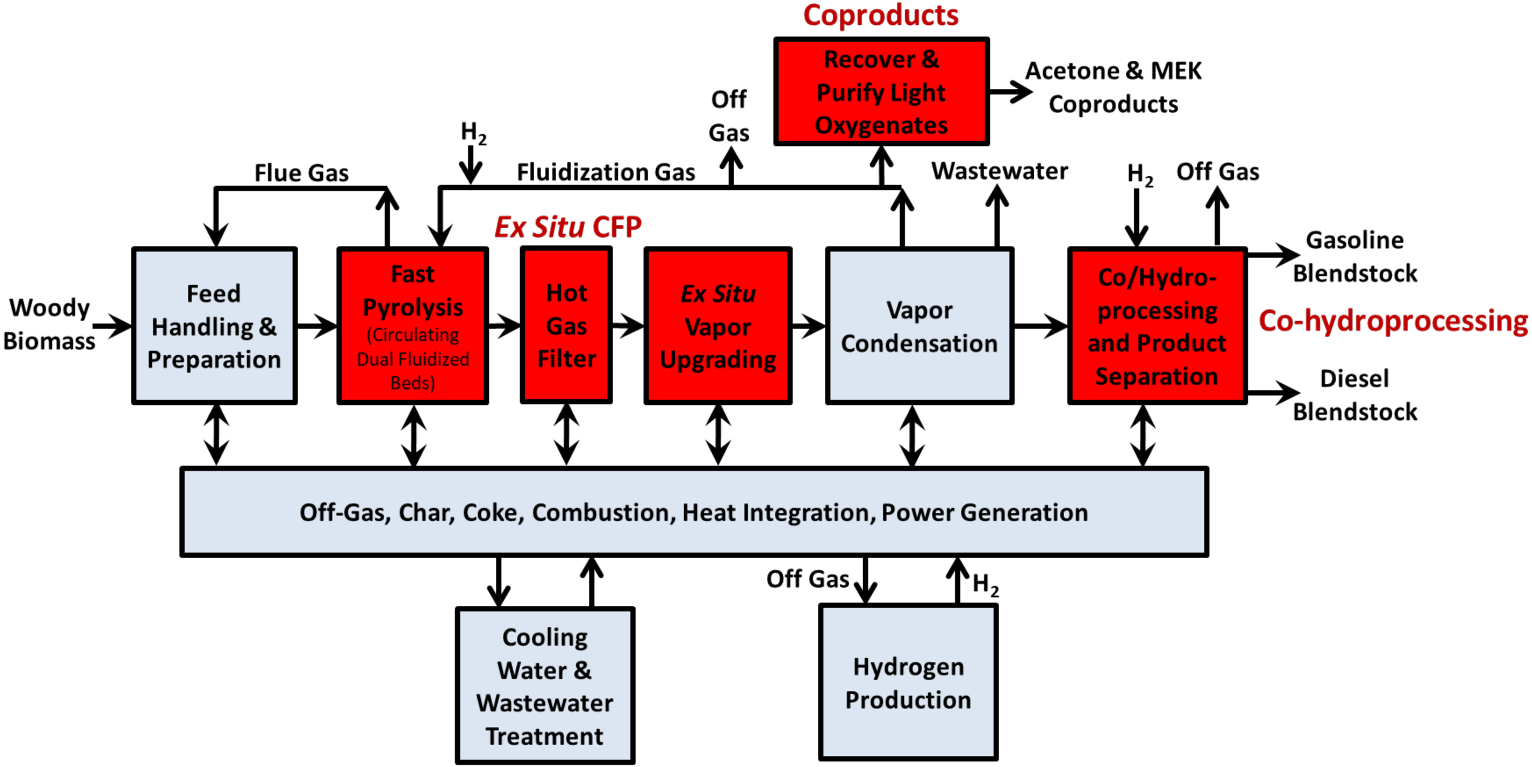
- DEI goals established by pooling resources with other TEA projects (includes Biochemical Analysis, Algae TEA, Strategic Support)
- **FY25 DEI Milestone:** Joint manuscript with 1 or more MSI university collaborator (professor + student group) on TEA/LCA analysis

Progress and Outcomes

Progress & Outcomes

Simplified Block Flow Diagram: Fixed Bed *Ex Situ* CFP

Background Information for Fixed Bed *Ex Situ* CFP

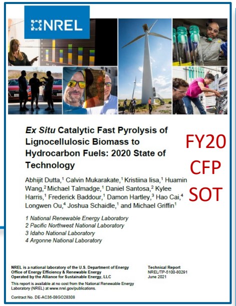


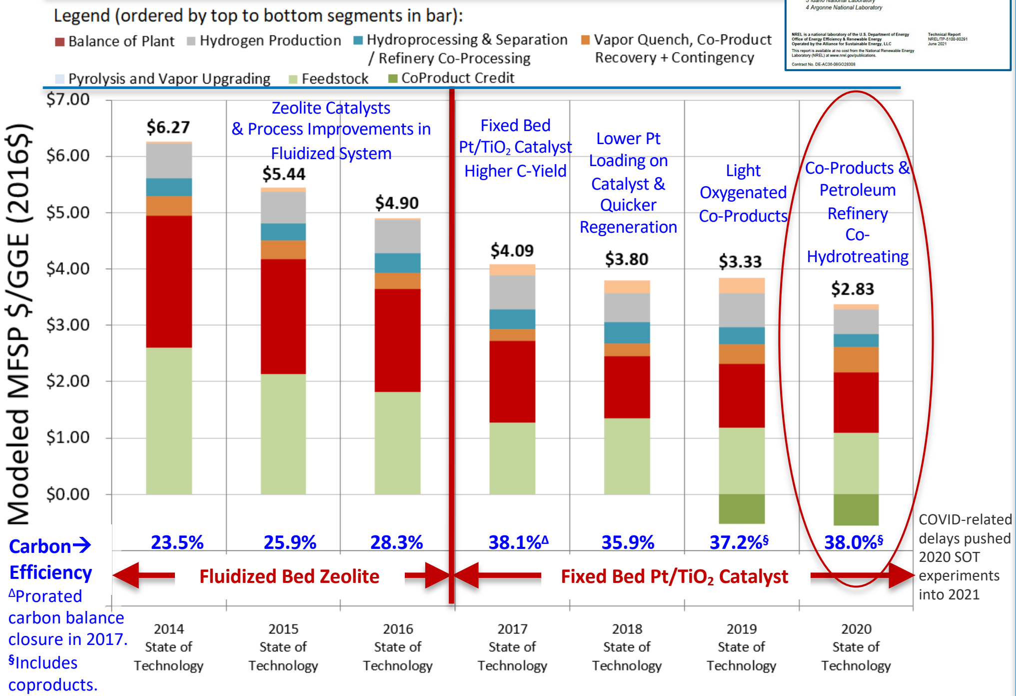
FY20 State of Technology report available at: https://www.nrel.gov/docs/fy21osti/80291.pdf

FY21 Closeout of CFP using Pt/TiO_2 Catalyst

Final modeling of 2021 bench-scale results showed that a fuel cost of <$3/GGE[1] and >75%[2] GHG reduction possible if scale-up is successful.

1: https://www.nrel.gov/docs/fy21osti/80291.pdf; 2: https://greet.es.anl.gov/files/2020_update_renewable_hc_fuel





CFP: Catalytic Fast Pyrolysis; **SOT:** State of Technology; **MFSP:** Minimum Fuel Selling Price; GGE: Gallon Gasoline Equivalent

Key Closeout Conclusions:

- Extensive *risk assessment* jointly with **experimental project (WBS 2.3.1.314)**
- Did not proceed with pilot scale-up in 2022 based on significant risks associated with the introduction of hydrogen within currently available pilot equipment
- Further R&D necessary for maturity / scale-up of coproducts recovery

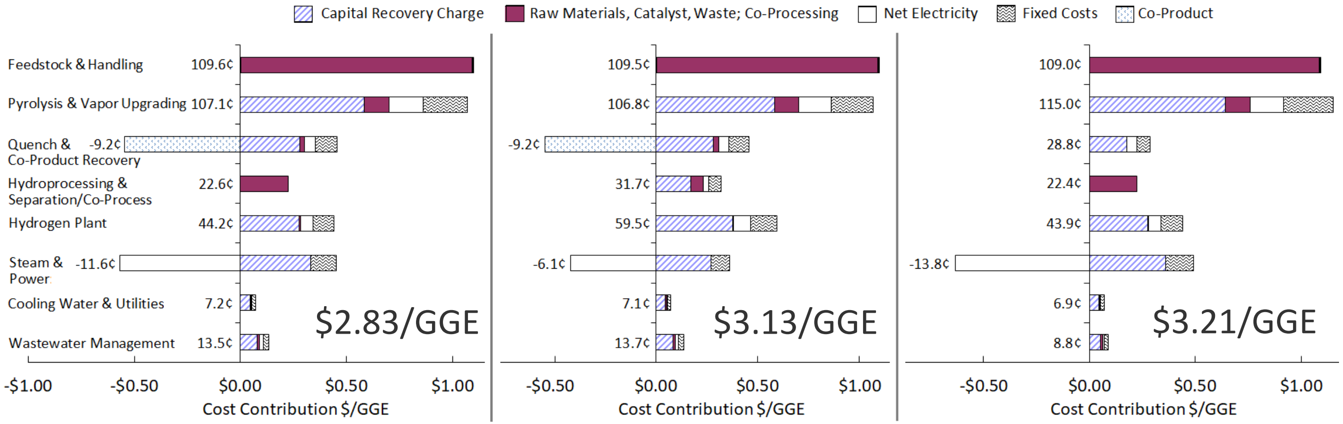
Future of this pathway:

- Technology remains promising; high fuel yield & selectivity to coproducts
- Continue to explore interested commercial entities to help address scale-up challenges

Progress & Outcomes

Closeout TEA/LCA Article for Fixed Bed *Ex Situ* CFP

Comparative analysis of configurations with different coproducts, hydrogen source options, and potential refinery co-hydroprocessing on costs and GHG emissions



Hydroprocessing	Co-HT at refinery	Standalone HT	Co-HT at refinery
Coproducts	Acetone & MEK	Acetone & MEK	No chemicals
Electricity	From excess energy	From excess energy	From excess energy
MFSP ($/GGE)	2.83	3.13	3.21
GHG Reduction*	77%	96%	62%

*GHG reduction over petroleum gasoline (93 gCO_2e/MJ); **MFSP:** Minimum Fuel Selling Price; **HT:** Hydrotreating

Quantified effects of:

- *Coproducts on cost and GHG emissions*
- *Refinery coprocessing on costs (this initial assessment with no significant added equipment expenses at refinery)*
- *Hydrogen source & significant impact on GHG emissions*

Dutta et al., Chemical Engineering Journal 451 (2023) 138485, https://doi.org/10.1016/j.cej.2022.138485 (multi-lab effort)

Progress & Outcomes

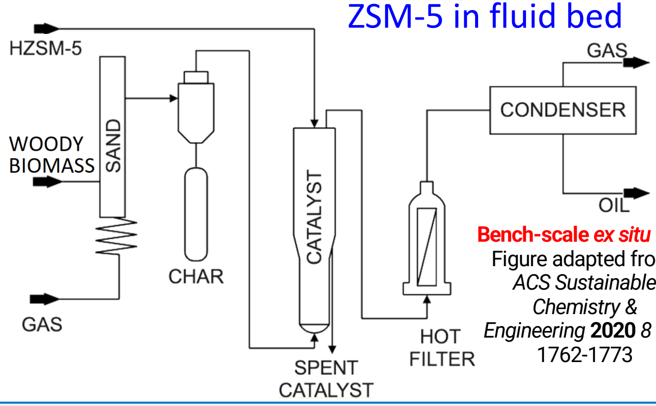
Understanding CFP & Hydrotreating towards SAF

Catalytic Fast Pyrolysis

Hydrotreating

Bench-scale experiments

ZSM-5 in fluid bed



Bench-scale *ex situ* CFP Figure adapted from: *ACS Sustainable Chemistry & Engineering* **2020** *8* (4), 1762-1773

Bench-scale hydrotreating Figure adapted from: *Iisa et al., 2022.* https://www.nrel.gov/docs/fy22osti/82696.pdf

March 2023 Analysis (*preliminary*) of Experimental Results showing the Impact of Varying CFP Oil Oxygen Content, followed by Standalone Hydrotreating

See backup slide 49 for additional information

Oxygen in CFP Oil	17%	20%	22%
CFP C-Efficiency (%)[1]	26	30	31
HT C-Efficiency (%)[2]	91	92	89
MFSP ($/GGE)[3]*	6.1-7.5	5.7-6.9	5.3-6.5
GHG Reduction (%)[4]	84	78	75

[1] Higher yields possible with optimization; C-efficiency values include condensable vapors in our *ex situ* CFP system; ZSM-5 catalyst used. Variations in yields with changes in CFP-oil oxygen content are consistent with expectations.

[2] NiMoS/Al_2O_3 catalyst. ~50% product is in the SAF range, meeting key jet fuel specs

[3] Modeled *Minimum Fuel Selling Price* (MFSP) in 2016$, with ±10% variation

[4] Approximate GHG reduction over petroleum gasoline (93 g CO_2e/MJ) with coproduct electricity from usable excess energy not converted to liquid fuels.

*Credits and incentives not included

Ongoing New Work on Refinery Integration & SAF

Hydroprocessing

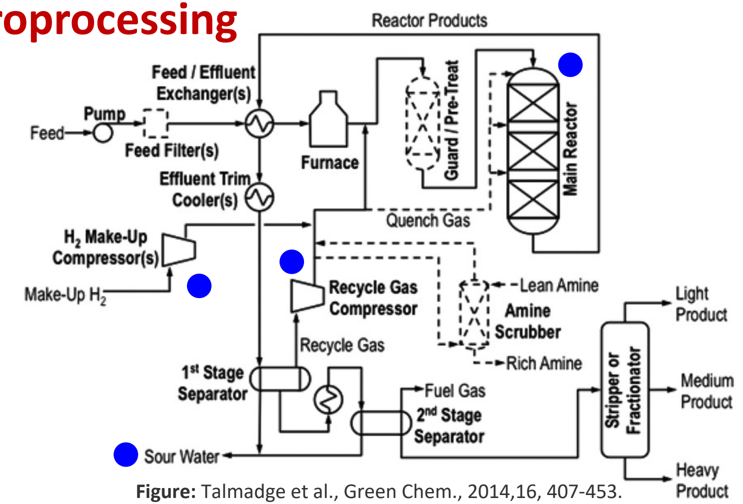


Figure: Talmadge et al., Green Chem., 2014,16, 407-453.

Working with KBR to ***assess risks and processing cost impacts*** from the introduction of CFP biocrudes in refineries

- Initial NREL modeling with hydrotreating
- Will expand other relevant refinery units

Assessments will be reported in FY24 design report and other publications

KBR subcontract

Enable prediction of ***SAF quality specifications*** in our process models: Facilitate achieving SAF requirements

	Density	LHV	Flash Point
	g/cm3	MJ/kg	°C
Specification	775-840	>42.8	>38
Sample 1 (ZSM-5 CFP Oil)	834	43	50
Sample 2 (Pt/TiO_2 CFP Oil)	833	43	47
Avg. abs. % error for 3 best predictions	0.47	0.11	3.8

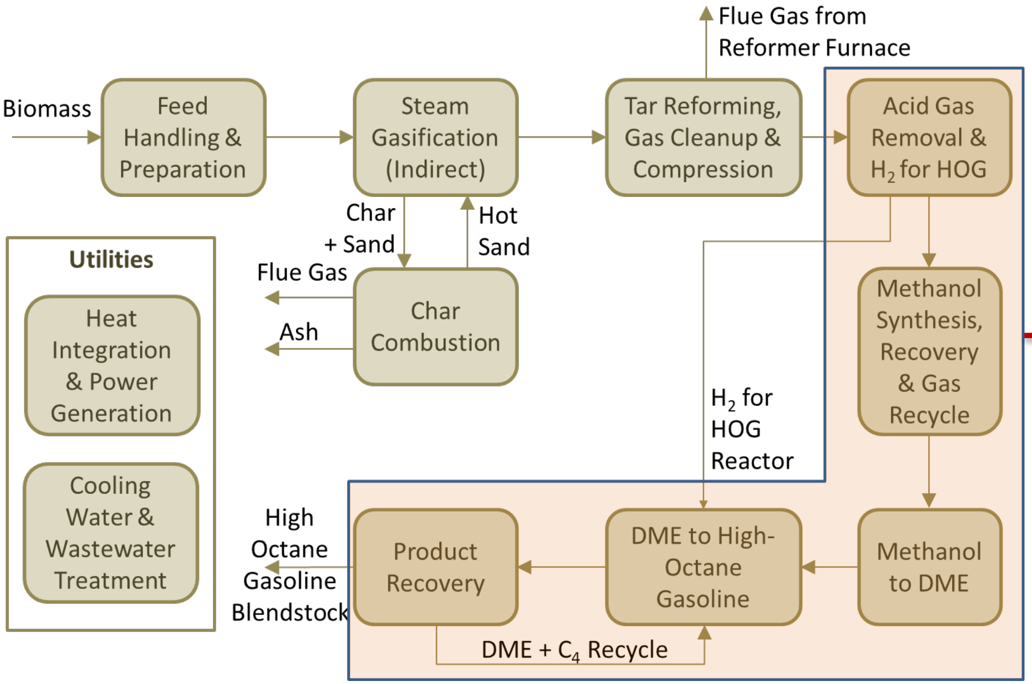
Samples 1 & 2 predictions from detailed speciation (>60 compounds each) of SAF range fuel from CFP oil hydrotreating. *Journal article submitted*, under review.

Experimental data: https://www.gti.energy/wp-content/uploads/2022/05/08-tcbiomass2022-Presentation-Kristiina-lisa.pdf

Subcontracts/Collaboration: Suphat Watanasiri, NIST

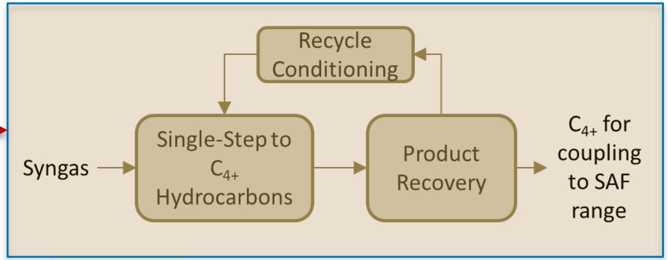
Flow Diagrams: 3-Steps to HOG vs. 1-Step to C_{4+}

2014-2021; closeout after 2021 SOT assessment



3-Steps to High-Octane Gasoline

Beginning 2021, after Go/No-Go 06/2021 assessment to determine whether 1-step approach can be viable



1-Step to C_{4+} Hydrocarbons*

Commercial methanol synthesis and methanol dehydration catalysts ($Cu/ZnO/Al_2O_3$ + γ-Al_2O_3, termed "CZA+A") positioned upstream of Cu/BEA

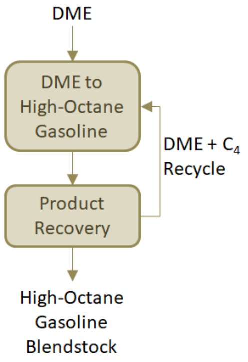
C_{4+} to SAF experiments in 2023*; TEA/LCA will follow

*Details in presentation by Dan Ruddy (WBS 2.3.1.305)

HOG: High Octane Gasoline; **SOT:** State of Technology; **SAF:** Sustainable Aviation Fuel

Progress & Outcomes

Closeout of 3-Step Syngas to High-Octane Gasoline



Research progress

- ***Ongoing work with industry towards commercial application***
- 2021 highlights (DME to HOG)
  - Reduced aromatics formation
  - Tested in larger bench scale reactor
  - Lower temperature for Cu/BEA catalyst regeneration

Biofpr

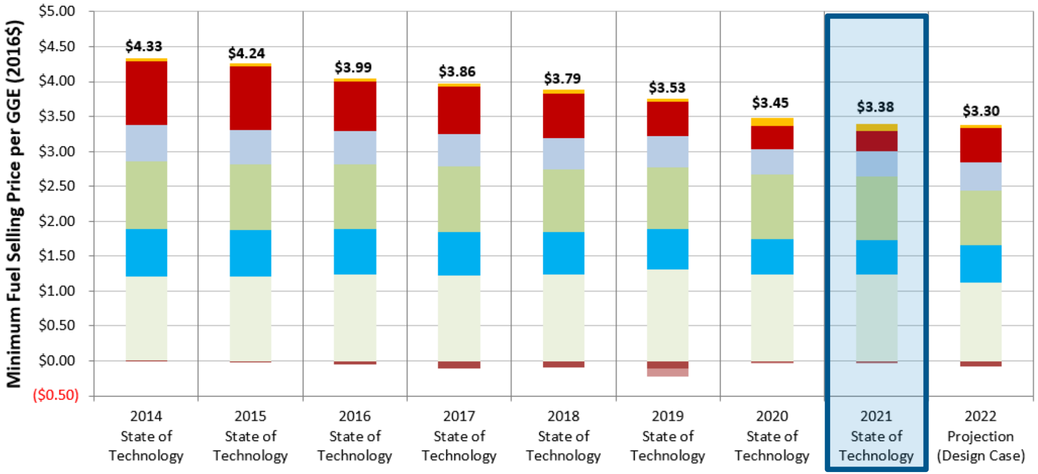
A separations and purification process for improving yields and meeting fuel contaminant specifications for high-octane gasoline produced from dimethyl-ether over a Cu/BEA catalyst

Abhijit Dutta, Daniel A. Ruddy, Connor P. Nash, Kylee Harris, Earl D. Christensen, Daniel P. Dupuis, Eric C.D. Tan, Catalytic Carbon Transformation & Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, USA

Received April 15 2022; Revised July 8 2022; Accepted July 11 2022;
View online August 10, 2022 at Wiley Online Library (wileyonlinelibrary.com);
DOI: 10.1002/bbb.2416; *Biofuels, Bioprod. Bioref.* 16:1469–1477 (2022)

https://doi.org/10.1002/bbb.2416

Published journal article based on recent model updates & related understanding of separations and recycle in 3-step process.



- LPG Coproduct Credit
- Hydrocarbon Product Separation
- Hydrocarbon Synthesis
- Acid Gas Removal, Methanol Synthesis and Methanol Conditioning
- Synthesis Gas Clean-up (Reforming and Quench)
- Gasification
- Feedstock
- Balance of Plant

>80% GHG reduction over petroleum-derived gasoline*

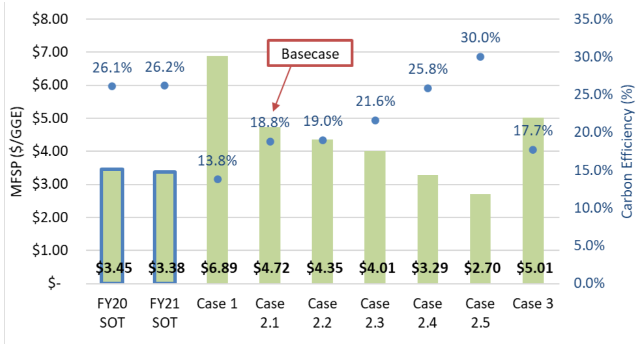
FY21 HOG SOT

References: Nature Catalysis, Vol 2, pages 632–640 (2019); https://www.nrel.gov/docs/fy22osti/81178.pdf; *https://publications.anl.gov/anlpubs/2022/04/174598.pdf

Additional information under : WBS 2.3.1.305 Upgrading of C1 Building Blocks
HOG: High-Octane Gasoline; **DME:** Dimethyl Ether;
SOT: State of Technology

1-Step Syngas-to-Hydrocarbons & Future Towards SAF

Go/No-Go Q3-Q4 2021



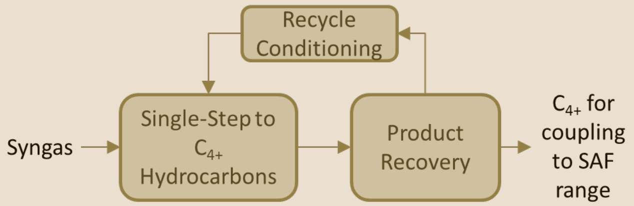
Initial sensitivity analysis to assess potential of 1-step STH process

2021 go/no-go TEA led by Kylee Harris

Process modeling to determine industrially relevant operating conditions → Further experiments at some of the identified operating conditions → Initial TEA to provide preliminary estimates of Minimum C4+ Hydrocarbon Selling Price (MHSP) and overall carbon efficiency

FY23 Q1: Initial TEA using bench-scale powdered catalyst results

Preliminary **MHSP of <$3/GGE** ($2.61/GGE initial estimate, will likely change as we refine the TEA); **>31% overall carbon efficiency** possible. Based on these yields, our current rough estimates project **>80% GHG reduction** for C4+ hydrocarbons on a GGE basis because yields are better than the 3-step HOG process.

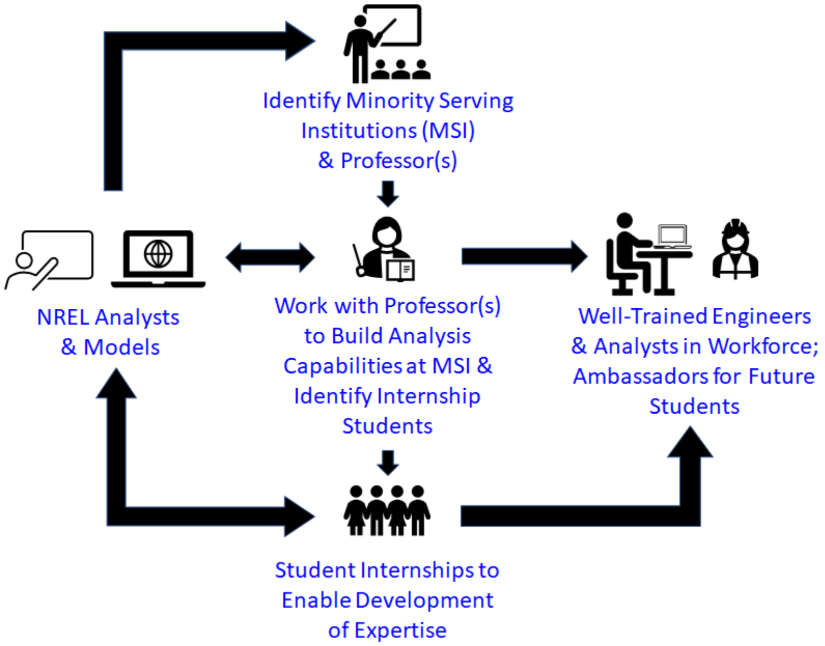


Next Steps: (a) FY23 Q3 milestone to refine TEA/LCA, (b) C_{4+} hydrocarbons to SAF, TEA/LCA after FY23 Q3 experiments

STH: Syngas to Hydrocarbons (C4+); **MHSP:** Min.(C4+) Hydrocarbon Selling Price; **GGE:** Gallon Gasoline Equivalent; **HOG:** High Octane Gasoline

Additional information under : WBS 2.3.1.305 Upgrading of C1 Building Blocks

DEI Progress



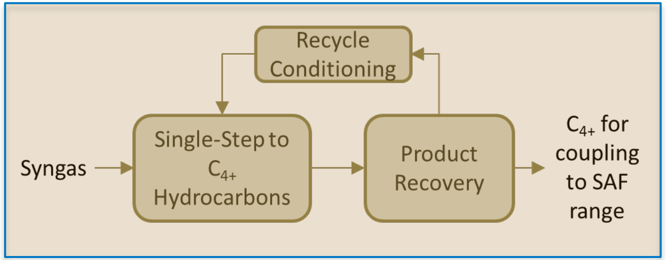
- In conversation with MSI for interns to initiate collaborative work
- Working towards goal of joint work products (and publication) by 2025

Impact

Impact on Core Experimental Research

Important role during transition to 1-step hydrocarbon process

- Helped narrow broad parameter space by providing potentially industrially relevant operating conditions and compositions for experiments



Guidance for relevant unit operations & conditions for processing pyrolytic biocrudes in refineries

- Feedback loop with researchers to allow exploration of processing options appropriate for different qualities of biocrudes
  - Quantification of process impacts
  - Advance model predictions through effective experiments
    - Help fill key gaps via modeling to inform stakeholders

Enable SAF & low-emission liquid fuels via pyrolytic and syngas conversion.
Provide inputs for *future scale-up, risk assessments; metrics for cost, GHG, technical targets* to enable successful research outcomes.

Impact

Inform and Enable Industry – Use Relevant Feedback

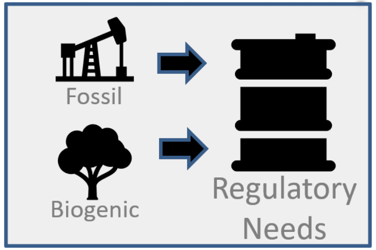
Direct Collaboration with Industry Partners

Leverage Knowledge & Modeling Capabilities from BETO Research

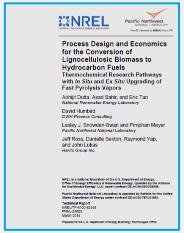
- ExxonMobil CRADA
- Alder Fuels

Other industrial entities (not listed) engaged via experimental projects

Facilitate Biogenic Carbon in Fuels and Products via Detailed Analysis



Publications to Disseminate Knowledge & Learnings


Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels
Thermochemical Research Pathways with *In Situ* and *Ex Situ* Upgrading of Fast Pyrolysis Vapors

Abhijit Dutta, Asad Sahir, and Eric Tan
National Renewable Energy Laboratory

David Humbird
DWH Process Consulting

Lesley J. Snowden-Swan and Pimphan Meyer
Pacific Northwest National Laboratory

Jeff Ross, Danielle Sexton, Raymond Yap, and John Lukas
Harris Group Inc.

- Detailed design reports
- State of Technology updates
- Journal articles

Solicit and Use Critical Review & Comments for Relevance

Other Products

- Software records for **detailed models** – available for licensing
- **Patents**/applications (led by experimental team)

Sample Models Publicly Available

https://www.nrel.gov/extranet/biorefinery/aspen-models/

NREL Transforming ENERGY

Biorefinery Analysis Process Models

Download and use by stakeholders, including academia and industry

List of publications, reports etc. since 2021 review is included in the Additional Slides section

Impact

Facilitate Broader Impact Analysis

Focus areas
- Diesel hydrotreaters (diesel mode) *70 BGal/yr*
- Distillate and/or gas oil hydrocrackers (jet mode) *37 BGal/yr*
- Fluid catalytic crackers (fuels and chemicals mode) *85 BGal/yr*

200 BGal/yr with flexibility to optimize and incorporate new technology.

Refinery Optimization Modeling

Experimental Data on Co-Processing and Standalone Upgrading

Hydroprocessing – Kristiina Iisa 2.3.1.314

Fluid Catalytic Cracking – Calvin Mukarakate, Reinhard Seisar 3.4.3.306-308

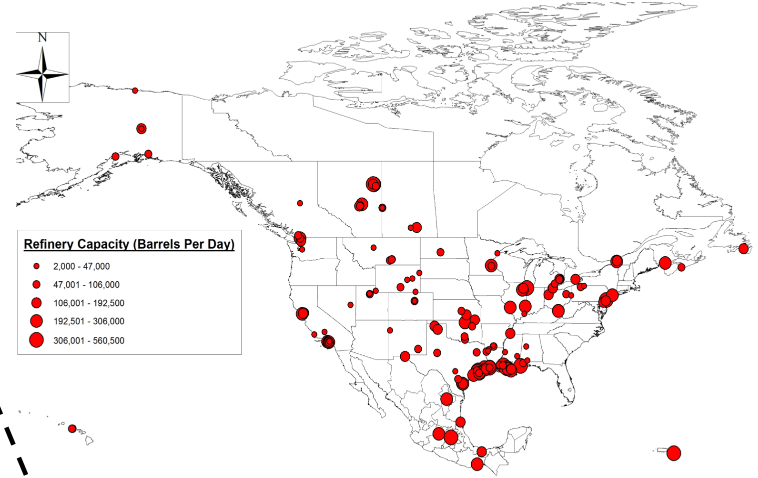
TEA Modeling for Processing in Diesel Hydrotreater (DHT), Hydrocracker (HCU) and other refinery units

TC Analysis – Abhijit Dutta 2.1.0.302

Aspen PIMS® Refinery Optimization Modeling with Bio-Intermediates and Bio-Blendstocks

Catalytic Upgrading – Mike Griffin 2.3.1.314

Bioeconomy Optimization Modeling



Bioeconomy Resource Optimization with US Refinery Network

Strategic Analysis – Ling Tao 4.1.1.30

BSM - Emily Newes 4.1.2.32

Work led by Michael Talmadge

Impact

Leverage Models for Other Research Projects

Published Articles Leveraging Knowledge/Models from this Project

Analysis for Marine Fuels

Environmental Science & Technology

pubs.acs.org/est Article

Techno-economic Analysis of Sustainable Biofuels for Marine Transportation

Shuyun Li,[⊥] Eric C. D. Tan,[*,⊥] Abhijit Dutta, Lesley J. Snowden-Swan, Michael R. Thorson, Karthikeyan K. Ramasamy,[*] Andrew W. Bartling, Robert Brasington, Michael D. Kass, George G. Zaimes, and Troy R. Hawkins

Cite This: *Environ. Sci. Technol.* 2022, 56, 17206−17214 Read Online

https://doi.org/10.1021/acs.est.2c03960

Analysis for FCIC

Modeling and Analysis Biofpr Biofuels Bioproducts & Biorefining

A simplified integrated framework for predicting the economic impacts of feedstock variations in a catalytic fast pyrolysis conversion process

Matthew R. Wiatrowski, **Abhijit Dutta**, Catalytic Carbon Transformation and Scale-up Center, National Renewable Energy Laboratory, Golden, CO, USA
M. Brennan Pecha, **Meagan Crowley**, **Peter N. Ciesielski**, Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO, USA
Daniel Carpenter, Catalytic Carbon Transformation and Scale-up Center, National Renewable Energy Laboratory, Golden, CO, USA

Received July 23 2021; Revised October 30 2021; Accepted November 02 2021;
View online November 26, 2021 at Wiley Online Library (wileyonlinelibrary.com);
DOI: 10.1002/bbb.2319; *Biofuels, Bioprod. Bioref.* 16:403–412 (2022)

https://doi.org/10.1002/bbb.2319

fcic FEEDSTOCK-CONVERSION INTERFACE CONSORTIUM U.S. DEPARTMENT OF ENERGY

Fuel Properties

Fuel 318 (2022) 123550

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

ELSEVIER

Short communication

Model-based compositional predictions for a differential scanning calorimetry/thermogravimetric analysis-mass spectrometry system used for heat of vaporization measurements

Abhijit Dutta[*], Gina M. Fioroni, Earl D. Christensen, Cameron K. Hays, Lisa Fouts, Suphat Watanasiri, Robert L. McCormick

National Renewable Energy Laboratory, 15013 Denver West Parkway, Golden, CO 80401, USA

https://doi.org/10.1016/j.fuel.2022.123550

Summary

Enabled productive research outcomes through TEA and sustainability modeling

- **Closeout of High-Octane Gasoline and Pt/TiO_2 CFP pathways**
  - Journal articles published, in addition to SOT reports
- Significant feedback to experimental research team for **pivots to next focus areas**
  - Process modeling-informed experiments and TEA for 1-step syngas to hydrocarbons
  - Informing experiments and identifying bottlenecks for pyrolytic biocrudes hydroprocessing
    - Integrating SAF property predictions to facilitate SAF from the conversion processes

Future Work

- Continue to model and inform ***syngas to hydrocarbons*** **pathway research towards SAF**, working in tandem with experimental research
- Continue **detailed modeling and assessment of refinery processing** of pyrolytic biocrudes
  - Work with industry experts' feedback to develop a design report to enable stakeholders
- Advance the outlined **DEI plan**

Quad Chart Overview

Timeline

- Project start date: October 1, 2022
- Project end date: September 30, 2025

	FY22 Costed	Total Award
DOE Funding	*$726k (actual costed)*	$2,100k ($700k each for FY23, FY24, and FY25)

This is an analysis project. TRL is N/A for Modality #5: strategic, market, and techno-economic analysis.

TRL start and end of the related core experimental research projects are presented under WBS# 2.3.1.305 (Dan Ruddy) and WBS# 2.3.1.314 (Mike Griffin).

Project Goal

To inform and guide R&D priorities for thermal and catalytic conversion processes through process-design-based TEA and sustainability analysis. Specific conversion pathways of focus are upgrading of pyrolytic biocrude intermediates and syngas to Sustainable Aviation Fuels (SAF) & other heavy-duty fuels.

End of Project Milestone

Final draft of a broad-scope design report and/or major publication covering multiple conversion options and product/fuel targets for the thermocatalytic conversion of biomass and waste feedstocks. Criteria: maximization of SAF with increases of at least 10% (e.g., using hybrid pyrolysis and syngas conversion approaches) while maintaining a 70% GHG reduction over petroleum derived fuels.

Funding Mechanism

National laboratory project funded by BETO.

Acknowledgements

DOE BETO for funding and support

NREL (includes subcontracts & recent-past contributors)

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- Mike Griffin
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- Jesse Hensley
- David Humbird
- Kristina Iisa
- Kim Magrini
- Bob McCormick
- Calvin Mukarakate
- Connor Nash
- Claire Nimlos
- Mark Nimlos
- Hakan Olcay
- Kellene Orton
- Dan Ruddy
- Eugene Paulechka
- Josh Schaidle
- Reinhard Seiser
- Avantika Singh
- Michael Talmadge
- Eric Tan
- Suphat Watanasiri
- Matt Wiatrowski
- Nolan Wilson
- Geetanjali Yadav
- Matt Yung
- Thermo-catalytic conversion team
- Biorefinery analysis team

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- Yuan Jiang
- Aye Meyer
- Steve Phillips
- Lesley Snowden-Swan
- Huamin Wang

INL

- Damon Hartley
- David Thompson

ANL

- Hao Cai
- Longwen Ou

NIST-TRC

- Chris Muzny
- Vladimir Diky

Feedstock Interface (FCIC)

ChemCatBio

Consortium for Computational Physics and Chemistry (CCPC)

Separations Consortium

Co-Optima

ExxonMobil

Alder Energy

Johnson Matthey

Petrobras

Thank you

www.nrel.gov

NREL/PR-5100-85397

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NREL Transforming ENERGY

Additional Slides

Responses to Previous Reviewers' Comments

1-3 significant questions/criticisms from the previous reviewers' comments that can be addressed within the scope of this project.

Comment 1: Key question for the management is how to get more engagement with broader oil and gas suppliers as their models are quite valuable and feedback from industry will always provide improvements?

Response: We have and will continue to engage with relevant industrial entities to maintain relevance and usefulness of our work for stakeholders. This FY23 presentation lists some of industrial entities (as did the FY21 presentation). We plan broad industrial outreach for our next significant design report draft planned for March 2024; we will be transparent about the specifics of that outreach in our publication (as in our previous reports).

Comment 2: Some progress has been made in identifying and quantifying for all CFP pathways and products that can be integrated within a traditional refinery environment with the completion of the stand-alone case. No preliminary work was presented yet on the co-processing case.

Response: We have since published our co-processing analysis and related results (after the FY21 peer review). Details are available in our State of Technology report (https://www.nrel.gov/docs/fy21osti/80291.pdf), and a journal article that presented a comparative analysis to show the impacts of standalone vs co-processing approaches, as well as the inclusion of coproducts (Chemical Engineering Journal, Vol. 451, 2023, 138485).

Comment 3: The LP (linear programming) work using ASPEN PIMS should be used in tandem with this effort so that the impact is not too unit specific.

Response: We included a slide in this presentation to show how our modeling work will interface with other broader analysis funded by BETO, including work under the Aspen PIMS framework.

Publications, Patents, Presentations, Awards, and Commercialization (1)

Commercialization efforts listed by experimental projects supported by this project

Publications:

- Dutta, A.; H. Cai; M.S. Talmadge; C. Mukarakate; K. Iisa; H. Wang; D.M. Santosa; L. Ou; D.S. Hartley; A.N. Wilson; J.A. Schaidle; M.B. Griffin. Model quantification of the effect of coproducts and refinery co-hydrotreating on the economics and greenhouse gas emissions of a conceptual biomass catalytic fast pyrolysis process. Chemical Engineering Journal. Volume 451, Part 1, 1 January 2023, 138485. https://doi.org/10.1016/j.cej.2022.138485.
- Li, S.; Tan, E.C.D.; Dutta, A.; Snowden-Swan, L.J.; Thorson, M.R.; Ramasamy, K.K.; Bartling, A.W.; Brasington, R.; Kass, M.D.; Zaimes, G.G.; Hawkins, T.R. Techno-economic Analysis of Sustainable Biofuels for Marine Transportation. Environ. Sci. Technol. 2022, 56, 17206−17214. https://doi.org/10.1021/acs.est.2c03960.
- Dutta, A.; Ruddy, D.A.; Nash, C.P.; Harris, K.; Christensen, E.D.; Dupuis, D.P.; Tan, E.C.D. A separations and purification process for improving yields and meeting fuel contaminant specifications for high-octane gasoline produced from dimethyl-ether over a Cu/BEA catalyst. BioFPR (2022). https://doi.org/10.1002/bbb.2416.
- Harris, Kylee, Connor Nash, Daniel Ruddy, Abhijit Dutta, Dan Dupuis, Earl Christensen, Alexander Rein, Eric Tan, Damon Hartley, Hao Cai, and Longwen Ou. 2022. High-Octane Gasoline From Lignocellulosic Biomass via Syngas and Methanol/Dimethyl Ether Intermediates: 2021 State of Technology. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-81178. https://www.nrel.gov/docs/fy22osti/81178.pdf.
- Dutta, Abhijit, Gina M. Fioroni, Earl D. Christensen, Cameron K. Hays, Lisa Fouts, Suphat Watanasiri, Robert L. McCormick. Model-based compositional predictions for a differential scanning calorimetry/thermogravimetric analysis-mass spectrometry system used for heat of vaporization measurements. Fuel 318 (2022) 123550. https://doi.org/10.1016/j.fuel.2022.123550.
- Wilson et al. Efficacy, economics, and sustainability of bio-based insecticides from thermochemical biorefineries. Green Chemistry, 2021. https://doi.org/10.1039/D1GC02956H
- Wiatrowski, MR; Dutta, A; Pecha, MB; Crowley, M; Ciesielski, PN; Carpenter, D. A simplified integrated framework for predicting the economic impacts of feedstock variations in a catalytic fast pyrolysis conversion process. Biofuels, Bioprod. Bioref. (2021). https://doi.org/10.1002/bbb.2319

Publications, Patents, Presentations, Awards, and Commercialization (2)

- Cai et al. Supply Chain Sustainability Analysis of Renewable Hydrocarbon Fuels via Indirect Liquefaction, Hydrothermal Liquefaction, Combined Algal Processing, and Biochemical Conversion: Update of the 2021 State-of-Technology Cases. April 2021. ANL/ESD-22/5 Rev. 1 174598. https://doi.org/10.2172/1862925.
- Dutta, Abhijit, Calvin Mukarakate, Kristiina Iisa, Huamin Wang, Michael Talmadge, Daniel Santosa, Kylee Harris, Frederick Baddour, et al. 2021. Ex Situ Catalytic Fast Pyrolysis of Lignocellulosic Biomass to Hydrocarbon Fuels: 2020 State of Technology. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-80291. https://www.nrel.gov/docs/fy21osti/80291.pdf.
- Harris, Kylee, Daniel Ruddy, Connor Nash, Abhijit Dutta, Daniel Dupuis, Eric Tan, Damon Hartley, and Hao Cai. 2021. High-Octane Gasoline from Lignocellulosic Biomass via Syngas and Methanol/Dimethyl Ether Intermediates: 2020 State of Technology. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-79986. https://www.nrel.gov/docs/fy21osti/79986.pdf.
- Eugene Paulechka; Vladimir Diky; Abhijit Dutta. 2021. Evaluation of Experimental and Predicted Vapor-Liquid Equilibrium Data for Systems Relevant to Biomass Fast Pyrolysis and Catalytic Upgrading . NIST Interagency/Internal Report (NISTIR) - 8357. NREL/TP-5100-78193. https://dx.doi.org/10.6028/NIST.IR.8357.
- Cai, H., L. Ou, M. Wang, R. Davis, A. Dutta, K. Harris, M. Wiatrowski, et al. 2021. 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. Lemont, IL: Argonne National Laboratory. ANL/ESD-21/1. https://doi.org/10.2172/1823113.

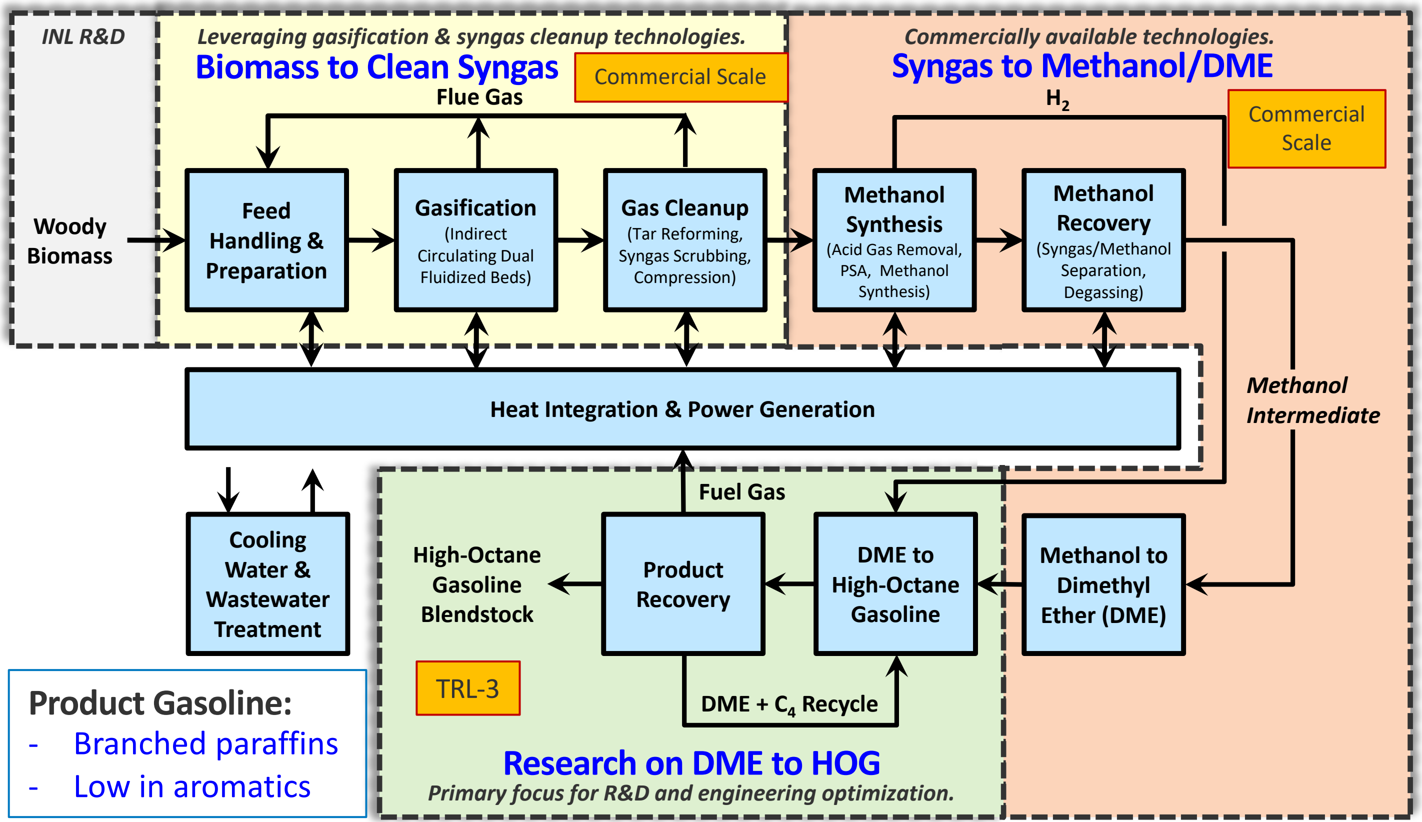
Presentations:

- Techno-Economic Analysis of Fixed Bed Ex-Situ Catalytic Fast Pyrolysis Using a Pt/TiO2 Catalyst for the Production of Fuels and Oxygenated Co-Products. Poster presentation at TC Biomass 2022. Dutta, A.; Mukarakate, C.; Iisa, K.; Wang, H.; Talmadge, M.; Santosa, D.; Harris, K.; Baddour, F.; Cai, H.; Ou, L.; Hartley, D.; Schaidle, J.A.; Griffin, M.
- Co-Hydrotreating of Catalytic Fast Pyrolysis Oils with Straight-Run Diesel. Presentation by Kristiina Iisa at TC Biomass 2022. Kristiina Iisa; Kellene Orton; Calvin Mukarakate; Abhijit Dutta; Joshua Schaidle; Michael Griffin; Luke Tuxworth; Mike Watson.

Additional content for conversion pathways

- High-Octane Gasoline (HOG)

Syngas to High-Octane Gasoline Conceptual Process



Product Gasoline:
- Branched paraffins
- Low in aromatics

Related Presentation

WBS 2.3.1.305

Upgrading of C1 Building Blocks

Commercialization-related engagements with industrial entities

Analysis includes use of waste material and CO_2

HOG: High-Octane Gasoline. **TRL:** Technology Readiness Level.

References: Nature Catalysis, Vol 2, pages 632–640 (2019); https://www.nrel.gov/docs/fy22osti/81178.pdf; https://www.nrel.gov/docs/fy15osti/62402.pdf

Syngas to High-Octane Gasoline State of Technology (1)

Processing Area Cost Contributions & Key Technical Parameters	Units	2014 SOT †	2015 SOT †	2016 SOT †	2017 SOT †	2018 SOT †	2019 SOT †	2020 SOT †	2021 SOT †	2022 Projection (Design Case)
Process Concept: Gasification, Syngas Cleanup, Methanol / DME Synthesis & Conversion to HCs		Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock	Woody Feedstock
C_5+ Minimum Fuel Selling Price (per Actual Product Volume) ▲	$ / Gallon	$4.31	$4.17	$3.85	$3.67	$3.66	$3.35	$3.22	$3.14	$3.22
Mixed C_4 Minimum Fuel Selling Price (per Actual Product Volume) ▲	$ / Gallon	$3.98	$3.91	N/A	N/A	N/A	$1.02	N/A	N/A	N/A
Minimum Fuel Selling Price (per Gallon of Gasoline Equivalent) ▲	$ / Gal GE	$4.33	$4.24	$3.99	$3.86	$3.79	$3.53	$3.45	$3.38	$3.30
Conversion Contribution (per Gallon of Gasoline Equivalent) ▲	$ / Gal GE	$3.13	$3.03	$2.76	$2.64	$2.56	$2.23	$2.21	$2.14	$2.18
Year for USD ($) Basis		2016	2016	2016	2016	2016	2016	2016	2016	2016
Total Capital Investment per Annual Gallon	$	$15.80	$15.94	$11.01	$11.54	$11.07	$11.07	$10.94	$10.85	$9.79
Plant Capacity (Dry Feedstock Basis)	Tonnes / Day	2,000	2,000	2,000	2,000	2,000	2,000	2,000	2,000	2,000
High-Octane Gasoline Blendstock (C_5+) Yield	Gallons / Dry Ton	36.2	36.4	51.4	50.0	51.4	51.6	55.1	55.6	56.0
Mixed C_4 Co-Product Yield	Gallons / Dry Ton	16.3	16.2	0.0	0.0	0.0	5.6	0.0	0.0	0.0
Feedstock										
Total Cost Contribution	$ / Gallon GE	$1.20	$1.21	$1.24	$1.22	$1.23	$1.31	$1.24	$1.23	$1.12
Capital Cost Contribution	$ / Gallon GE	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00
Operating Cost Contribution	$ / Gallon GE	$1.20	$1.21	$1.24	$1.22	$1.23	$1.30	$1.24	$1.23	$1.12
Feedstock Cost	$ / Dry US Ton	$60.58	$60.58	$60.58	$57.28	$60.54	$63.23	$63.23	$63.23	$60.54
Ash Content	wt % Ash	3.00%	3.00%	3.00%	3.00%	3.00%	1.75%	1.75%	1.75%	3.00%
Feedstock Moisture at Plant Gate	Wt % H_2O	30%	30%	30%	30%	30%	30%	30%	30%	30%
In-Plant Handling and Drying / Preheating	$ / Dry US Ton	$0.72	$0.70	$0.70	$0.69	$0.69	$0.69	$0.57	$0.57	$0.69
Cost Contribution	$ / Gallon	$0.01	$0.01	$0.01	$0.01	$0.01	$0.01	$0.01	$0.01	$0.01
Feed Moisture Content to Gasifier	wt % H_2O	10%	10%	10%	10%	10%	10%	10%	10%	10%
Energy Content (LHV, Dry Basis)	BTU / lb	7,856	7,856	7,856	7,856	7,856	7,933	7,930	7,930	7,856
Gasification										
Total Cost Contribution	$ / Gallon GE	$0.69	$0.67	$0.65	$0.62	$0.61	$0.58	$0.50	$0.49	$0.54
Capital Cost Contribution	$ / Gallon GE	$0.43	$0.41	$0.38	$0.35	$0.34	$0.33	$0.28	$0.27	$0.30
Operating Cost Contribution	$ / Gallon GE	$0.26	$0.26	$0.27	$0.28	$0.26	$0.25	$0.23	$0.22	$0.24
Raw Dry Syngas Yield	lb / lb Dry Feed	0.76	0.76	0.76	0.76	0.76	0.77	0.83	0.83	0.76
Raw Syngas Methane (Dry Basis)	Mole %	15.4%	15.4%	15.4%	15.4%	15.4%	15.4%	8.6%	8.7%	15.4%
Gasifier Efficiency (LHV)	% LHV	71.9%	71.9%	71.9%	71.9%	71.9%	72.3%	78.0%	78.5%	71.9%
Synthesis Gas Clean-up (Reforming and Quench)										
Total Cost Contribution	$ / Gallon GE	$0.96	$0.93	$0.94	$0.94	$0.89	$0.88	$0.93	$0.92	$0.78
Capital Cost Contribution	$ / Gallon GE	$0.51	$0.49	$0.46	$0.43	$0.41	$0.39	$0.40	$0.40	$0.36
Operating Cost Contribution	$ / Gallon GE	$0.45	$0.45	$0.48	$0.51	$0.48	$0.49	$0.53	$0.52	$0.42
Tar Reformer (TR) Exit CH_4 (Dry Basis)	Mole %	1.7%	1.7%	1.7%	1.7%	1.7%	1.7%	1.3%	1.3%	1.7%
TR CH_4 Conversion	%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%	80.0%
TR Benzene Conversion	%	99.0%	99.0%	99.0%	99.0%	99.0%	99.0%	99.0%	99.0%	99.0%
TR Tars Conversion	%	99.9%	99.9%	99.9%	99.9%	99.9%	99.9%	99.9%	99.9%	99.9%
Catalyst Replacement	% of Inventory / Day	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%	0.15%

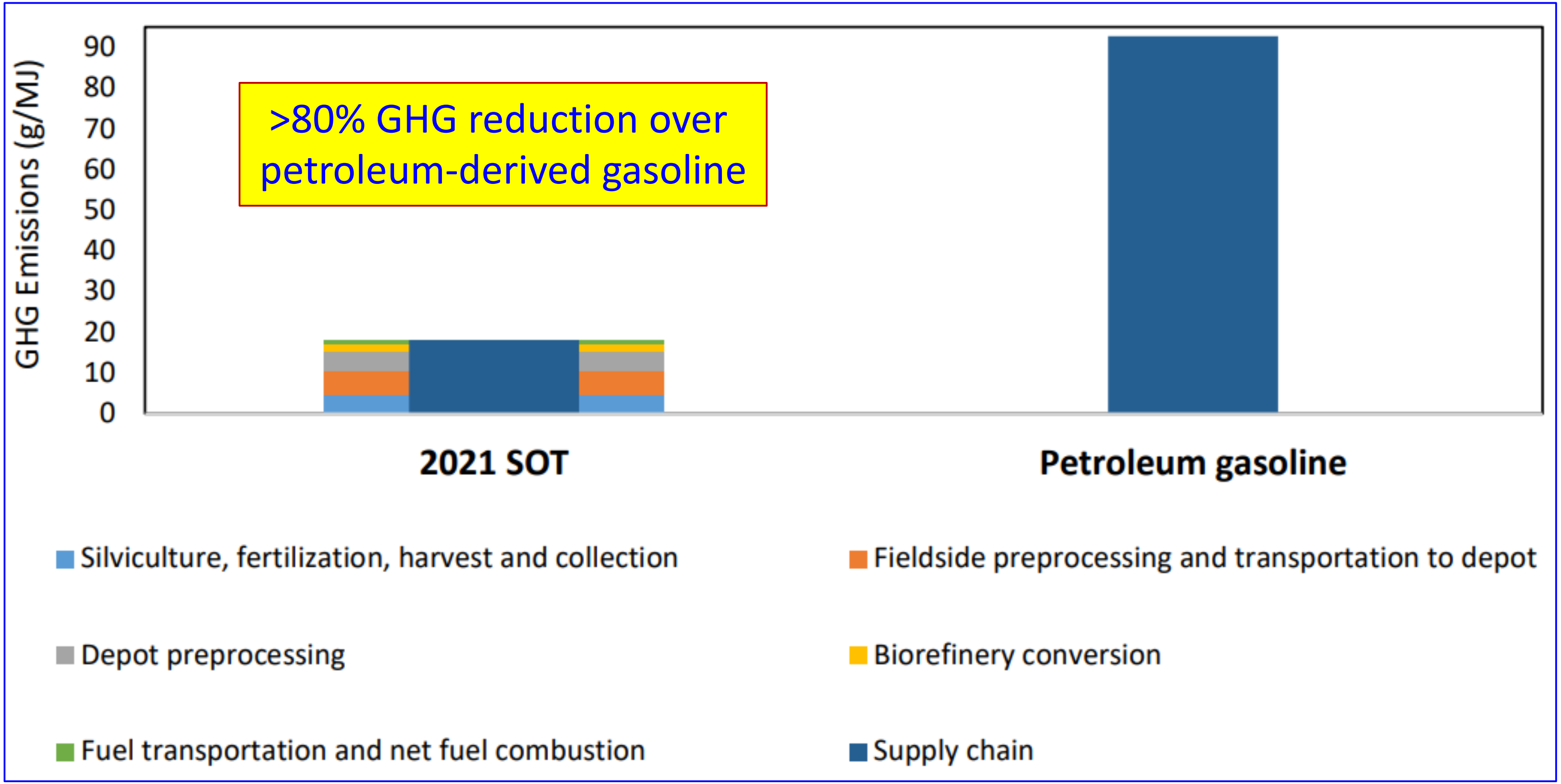
Reference: https://www.nrel.gov/docs/fy22osti/81178.pdf; †**SOT:** State of Technology.

Syngas to High-Octane Gasoline State of Technology (2)

Acid Gas Removal, Methanol Synthesis and Methanol Conditioning										
Total Cost Contribution	$ / Gallon GE	$0.52	$0.50	$0.47	$0.47	$0.45	$0.45	$0.36	$0.36	$0.40
Capital Cost Contribution	$ / Gallon GE	$0.35	$0.33	$0.30	$0.28	$0.28	$0.27	$0.20	$0.20	$0.24
Operating Cost Contribution	$ / Gallon GE	$0.17	$0.17	$0.17	$0.19	$0.18	$0.18	$0.15	$0.16	$0.16
Methanol Synthesis Reactor Pressure	psia	730	730	730	730	730	730	730	730	730
Methanol Productivity	kg / kg-cat / hr	0.7	0.7	0.8	0.8	0.8	0.7	0.8	0.8	0.7
Methanol Intermediate Yield	Gallons / Dry Ton	143	142	138	144	141	137	150	152	134
Hydrocarbon Synthesis										
Total Cost Contribution	$ / Gallon GE	$0.91	$0.91	$0.70	$0.67	$0.64	$0.49	$0.34	$0.29	$0.48
Capital Cost Contribution	$ / Gallon GE	$0.56	$0.56	$0.46	$0.44	$0.42	$0.34	$0.11	$0.11	$0.32
Operating Cost Contribution	$ / Gallon GE	$0.35	$0.35	$0.24	$0.23	$0.22	$0.16	$0.23	$0.17	$0.16
Methanol to DME Reactor Pressure	psia	145	145	145	145	145	145	169	169	145
Hydrocarbon Synthesis Reactor Pressure	psia	129	129	129	129	129	129	205	205	129
Hydrocarbon Synthesis Catalyst		Commercial Beta-Zeolite		NREL modified Beta-Zeolite with copper (Cu) as active metals for activity and performance improvement						
Hydrogen Addition to Hydrocarbon Synthesis		No H_2 Addition	Supplemental H_2 added to hydrocarbon synthesis reactor inlet to improve selectivity to branched paraffins relativete to aromatics							
Utilization of C_4 in Reactor Outlet via Recycle		0%	0%	100%	100%	100%	90%	97%	97%	100%
Single-Pass DME Conversion	%	15.0%	15.0%	19.2%	27.6%	38.9%	44.7%	43.4%	43.4%	40.0%
Overall DME Conversion	%	83%	85%	83%	88%	92%	88%	96%	96%	90%
Hydrocarbon Synthesis Catalyst Productivity	kg / kg-cat / hr	0.02	0.03	0.04	0.09	0.07	0.07	0.07	0.07	0.10
Carbon Selectivity to C_5+ Product	% C in Reactor Feed	46.2%	48.3%	81.8%	74.8%	72.3%	73.6%	72.1%	73.3%	86.7%
Carbon Selectivity to Total Aromatics (Including Hexamethylbenzene)	% C in Reactor Feed	25.0%	20.0%	4.0%	4.0%	8.0%	5.8%	3.3%	1.6%	0.5%
Carbon Selectivity to Coke and Pre-Cursors (Hexamethylbenzene Proxy)	% C in Reactor Feed	10.0%	9.3%	4.0%	4.0%	4.0%	2.9%	1.6%	1.6%	0.5%
Hydrocarbon Product Separation										
Total Cost Contribution	$ / Gallon GE	$0.04	$0.05	$0.05	$0.05	$0.05	$0.05	$0.11	$0.11	$0.05
Capital Cost Contribution	$ / Gallon GE	$0.03	$0.03	$0.04	$0.04	$0.04	$0.03	$0.06	$0.06	$0.03
Operating Cost Contribution	$ / Gallon GE	$0.01	$0.01	$0.01	$0.01	$0.01	$0.01	$0.05	$0.05	$0.01
LPG Coproduct Credit										
Total Cost Contribution	$ / Gallon GE	$0.00	$0.00	$0.00	$0.00	$0.00	($0.11)	($0.00)	($0.00)	$0.00
Balance of Plant										
Total Cost Contribution	$ / Gallon GE	$0.01	($0.02)	($0.05)	($0.11)	($0.09)	($0.11)	($0.03)	($0.02)	($0.07)
Capital Cost Contribution	$ / Gallon GE	$0.42	$0.40	$0.36	$0.34	$0.33	$0.29	$0.31	$0.30	$0.28
Operating Cost Contribution	$ / Gallon GE	($0.41)	($0.42)	($0.42)	($0.45)	($0.42)	($0.41)	($0.33)	($0.32)	($0.36)
Sustainability and Process Efficiency Metrics										
Carbon Efficiency to C_5+ Product	% C in Feedstock	19.3%	19.4%	25.2%	24.3%	25.5%	24.8%	26.1%	26.2%	27.9%
Carbon Efficiency to Mixed C_4 Co-Product	% C in Feedstock	7.0%	6.9%	0.0%	0.0%	0.0%	2.3%	0.0%	0.0%	0.0%
Overall Carbon Efficiency to Hydrocarbon Products	% C in Feedstock	26.3%	26.3%	25.2%	24.3%	25.5%	27.1%	26.1%	26.2%	27.9%
Overall Energy Efficiency to Hydrocarbon Products	% LHV of Feedstock	37.7%	37.7%	36.6%	35.1%	36.6%	39.6%	37.6%	37.9%	40.4%
Electricity Production	kWh / Gallon C_5+	11.7	11.8	7.9	8.4	8.1	7.6	12.2	11.9	7.0
Electricity Consumption	kWh / Gallon C_5+	11.7	11.8	7.9	8.5	8.1	7.6	12.2	11.9	7.0
Water Consumption	Gal H_2O / Gal C_5+	12.9	10.1	3.1	3.3	3.2	2.9	3.3	3.3	2.8

Reference: https://www.nrel.gov/docs/fy22osti/81178.pdf

HOG Pathway GHG Emissions

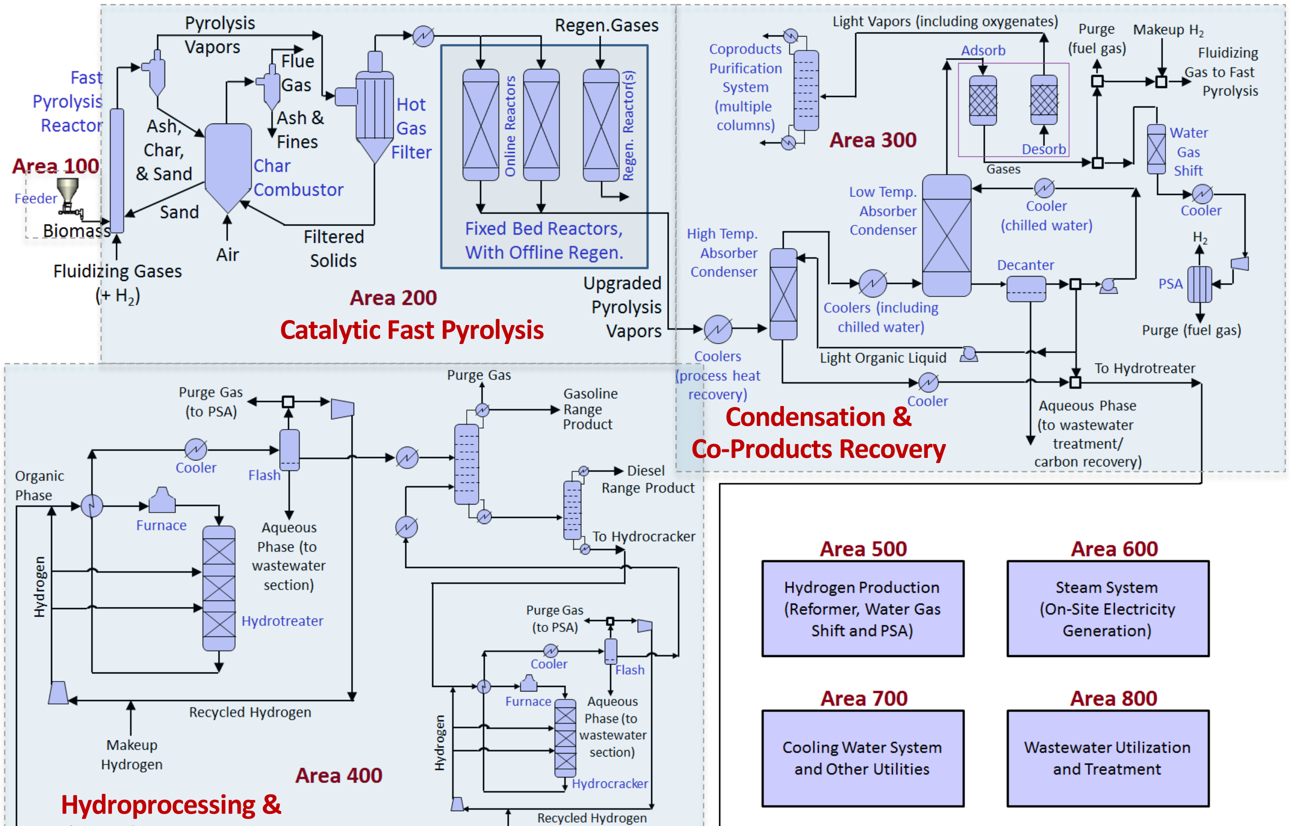


Reference: https://publications.anl.gov/anlpubs/2022/04/174598.pdf
2021 SOT: 2021 State of Technology for **High Octane Gasoline (HOG)** pathway

Additional content for conversion pathways

- Catalytic Fast Pyrolysis (CFP) FY20-21 Closeout
    - **Pt/TiO_2 catalyst in fixed bed** *ex situ* configuration

Catalytic Fast Pyrolysis (CFP) with Hydrotreating – Process Flow



References: Energy Environ. Science, 2018, 11, 2904;
https://www.nrel.gov/docs/fy21osti/80291.pdf

Area 100: Feedstock
Area 200: Fast Pyrolysis and Ex-Situ Catalytic Upgrading
Area 300: Condensation & Light Oxygenates Recovery
Area 400: Hydroprocessing & Fuel Product Separation
Area 500: Hydrogen Production from Off-Gases
Area 600: Steam System & Power Generation
Area 700: Cooling Water & Utilities
Area 800: Wastewater Treatment

Fixed Bed CFP with Hydrotreating State of Technology (1)

Processing Area Cost Contributions & Key Technical Parameters	Units	2014 SOT	2015 SOT	2016 SOT	2017 SOT[‡‡]	2018 SOT	2019 SOT	2020 SOT
Process Concept: Hydrocarbon Fuel Production via Ex Situ Upgrading of Fast Pyrolysis Vapors		**Clean Pine**	**Clean Pine**	**Clean Pine**	**Clean Pine**	**Clean Pine**	**50%Residues/50%Pine[††]**	**50%Residues/50%Pine[††]**
Year $ Basis		2016	2016	2016	2016	2016	2016	2016
Projected Minimum Fuel Selling Price[▲]	$/GGE*	$6.27	$5.44	$4.90	$4.09	$3.80	$3.33	$2.83
Conversion Contribution	$/GGE*	$3.66	$3.30	$3.08	$2.82	$2.44	$2.14	$1.74
Total Project Investment per Annual GGE	$/GGE-yr	$18.50	$16.46	$14.94	$12.17	$12.47	$13.53	$11.64
Plant Capacity (Dry Feedstock Basis)	metric tons/day	2,000	2,000	2,000	2,000	2,000	2,000	2,000
Total Gasoline Equivalent Yield	GGE/dry US ton	42	46	51	69	65	59	61
Diesel-Range Product Proportion (GGE* basis)	% of fuel product	15%	15%	15%	52%	52%	48%	50%
Feedstock								
Total Cost Contribution[††]	$ / GGE	$2.60	$2.14	$1.82	$1.27	$1.36	$1.18	$1.10
Capital Cost Contribution[††]	$ / GGE	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00
Operating Cost Contribution[††]	$ / GGE	$2.60	$2.14	$1.81	$1.27	$1.35	$1.18	$1.09
Feedstock Cost[‡‡]	$ / Dry US Ton	$109.01	$98.31	$92.70	$87.82	$87.82	$70.15	$67.03
Feedstock Moisture at Plant Gate	Wt % H_2O	10%	10%	10%	10%	10%	10%	10%
Feed Moisture Content to Pyrolyzer	wt % H_2O	10%	10%	10%	10%	10%	10%	10%
Energy Content (LHV, Dry Basis)	BTU / lb	8,000	8,000	8,000	8,000	8,000	7,900	7,900
Pyrolysis and Vapor Upgrading								
Total Cost Contribution	$ / GGE	$2.34	$2.03	$1.84	$1.46	$1.10	$1.14	$1.07
Capital Cost Contribution	$ / GGE	$0.95	$0.82	$0.74	$0.65	$0.60	$0.63	$0.58
Operating Cost Contribution	$ / GGE	$1.39	$1.21	$1.09	$0.80	$0.50	$0.51	$0.49
Ex Situ Reactor Configuration	reactor type	Fluidized Bed	Fluidized Bed	Fluidized Bed	Fixed Bed	Fixed Bed	Fixed Bed	Fixed Bed
Ratio of Online:Regenerating Fixed Bed Reactors	ratio	N/A	N/A	N/A	2:5	2:3	2:2	2:2
Gas Phase	wt % of dry biomass	35%	36%	34%	31%	35%	38%	42%
Aqueous Phase	wt % of dry biomass	25%	25%	24%	27%	22%	24%	20%
Carbon Loss	% of C in biomass	2.9%	2.9%	3.4%	2.9%	5.0%	4.4%	1.8%
Organic Phase	wt % of dry biomass	17.5%	18.6%	21.8%	28.3%	27.9%	23.2%	24.0%
H/C Molar Ratio	ratio	1.1	1.1	1.1	1.2	1.2	1.2	1.3
Oxygen	wt % of organic phase	15.0%	13.3%	16.8%	16.5%	18.6%	15.1%	16.6%
Carbon Efficiency	% of C in biomass	27%	29%	33%	42%	40%	35%	36%
Solid Losses (Char + Coke)	wt % of dry biomass	23%	21%	20%	14%	15%	14%	13%
Char	wt % of dry biomass	12.0%	11.0%	12.0%	10.4%	11.7%	11.6%	11.1%
Coke	wt % of dry biomass	11.0%	9.5%	8.3%	3.3%	3.7%	2.3%	1.7%
Vapor Quench, Co-Product Recovery								
Total Cost Contribution	$ / GGE	$0.35	$0.33	$0.28	$0.20	$0.22	$0.34	$0.45
Capital Cost Contribution	$ / GGE	$0.20	$0.19	$0.16	$0.12	$0.13	$0.22	$0.28
Operating Cost Contribution	$ / GGE	$0.15	$0.14	$0.12	$0.08	$0.09	$0.12	$0.18

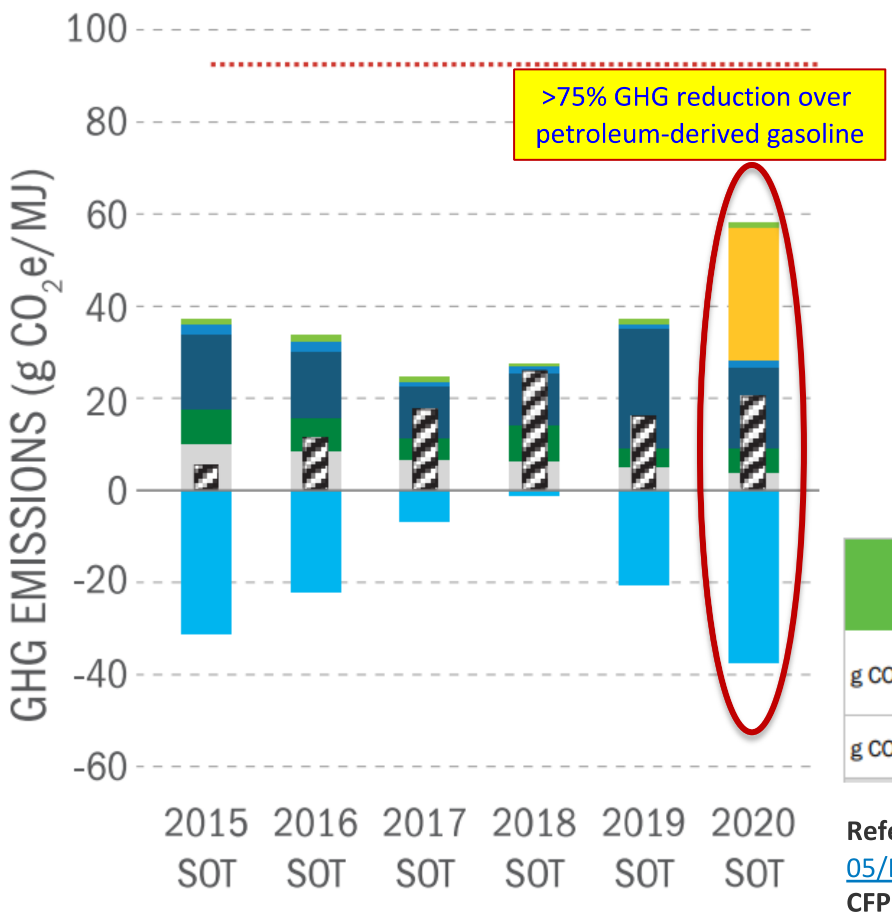
Reference: https://www.nrel.gov/docs/fy21osti/80291.pdf; **SOT:** State of Technology.

Fixed Bed CFP with Hydrotreating State of Technology (2)

Hydroprocessing & Separation / Refinery Co-Processing		2014 SOT	2015 SOT	2016 SOT	2017 SOT‡‡	2018 SOT	2019 SOT	2020 SOT
Total Cost Contribution	$ / GGE	$0.33	$0.31	$0.34	$0.35	$0.38	$0.30	$0.23
Capital Cost Contribution	$ / GGE	$0.17	$0.16	$0.18	$0.19	$0.20	$0.16	$0.00
Operating Cost Contribution	$ / GGE	$0.15	$0.14	$0.16	$0.16	$0.18	$0.14	$0.23
Carbon Efficiency of Organic Liquid Feed to Fuels	%	88.4%	89.5%	87.2%	91.0%	89.0%	93.5%	94.5%
Hydrotreating Pressure	psia	2,000	2,000	2,000	1,900	1,900	1,900	1,900
Oxygen Content in Cumulative Fuel Product	wt %	0.8%	0.8%	0.8%	0.6%	0.5%	0.5%	0.5%
Hydrogen Production								
Total Cost Contribution	$ / GGE	$0.61	$0.56	$0.60	$0.62	$0.51	$0.61	$0.44
Capital Cost Contribution	$ / GGE	$0.39	$0.36	$0.38	$0.41	$0.33	$0.39	$0.28
Operating Cost Contribution	$ / GGE	$0.22	$0.20	$0.22	$0.21	$0.18	$0.22	$0.16
Additional Natural Gas (NG) at the Biorefinery**	% of biomass LHV	0.3%	0.1%	0.2%	0.1%	0.3%	0.1%	0.1%
CoProducts								
Total Cost Contribution	$ / GGE						($0.52)	($0.55)
Capital Cost Contribution *	$ / GGE							
Operating Cost Contribution *	$ / GGE							
CoProduct Credit	$/GGE*						($0.52)	($0.55)
Balance of Plant								
Total Cost Contribution	$ / GGE	$0.04	$0.07	$0.03	$0.20	$0.23	$0.27	$0.09
Capital Cost Contribution	$ / GGE	$0.80	$0.71	$0.56	$0.43	$0.46	$0.45	$0.46
Operating Cost Contribution	$ / GGE	($0.76)	($0.64)	($0.54)	($0.23)	($0.23)	($0.18)	($0.37)
Electricity Production from Steam Turbine (credit included in op. cost above)	$/GGE*	($1.12)	($0.96)	($0.78)	($0.42)	($0.45)	($0.40)	($0.57)
Sustainability and Process Efficiency Metrics								
Fuel and Coproducts Yield by Weight of Biomass	% w/w of dry biomass	13.7%	15.0%	16.5%	22.2%	20.9%	22.5%	23.0%
Carbon Efficiency of Biomass to Fuels and Coproducts	% C in Feedstock	23.5%	25.9%	28.3%	38.1%	35.9%	37.2%	38.0%
Overall Carbon Efficiency to Liquid Hydrocarbon Fuels	% C in Feedstock	23.5%	25.9%	28.3%	38.1%	35.9%	33.0%	33.7%
Overall Energy Efficiency to Liquid Hydrocarbon Fuels	% LHV of Feedstock	30.5%	33.4%	37.1%	50.3%	47.2%	43.6%	45.1%
Electricity Production	kWh/GGE	21.0	18.0	14.7	8.0	8.7	7.8	10.6
Electricity Consumption (Entire Process)	kWh/GGE	12.7	11.0	9.6	6.4	7.5	7.4	5.9
Water Consumption in Conversion Process	gal H_2O/GGE	1.4	1.4	1.3	1.5	1.4	1.7	1.1

Reference: https://www.nrel.gov/docs/fy21osti/80291.pdf; **SOT:** State of Technology.

CFP Pathway GHG Emissions



	2015 SOT	2016 SOT	2017 SOT	2018 SOT	2019 SOT	2020 SOT
g CO_2e/MJ	6.0 (−94%)	11.4 (−88%)	17.7 (−81%)	26.4 (−72%)	16.2(−83%)	21 (−78%)
g CO_2e/GGE	738	1,402	2,171	3,234	1,985	2,538

Reference: https://bioenergykdf.net/sites/default/files/2022-05/BETO-2020-SOT_FINAL_5-11-22.pdf;
CFP: Catalytic Fast Pyrolysis

Additional content for conversion pathways

- Catalytic Fast Pyrolysis (CFP) FY23 TEA/LCA

  - **ZSM-5 CFP catalyst in fluid bed** *ex situ* configuration
  - Additional information supporting **Slide 19**

CFP-HT TEA (Slide 19) – Additional **Preliminary** Information

Financial assumptions consistent with FY20-21 State of Technology report*

Description of Assumption	Assumed Value
Cost year	2016
Internal rate of return on equity	10%
Plant financing by equity/debt	40%/60% of total capital investment
Plant life	30 years
Income tax rate	21%
Interest rate for debt financing	8.0% annually
Term for debt financing	10 years
Working capital cost	5.0% of fixed capital investment (FCI) (excluding land purchase cost)
Depreciation schedule	7-year MACRS [a] schedule [9]
Steam plant depreciation	20-year MACRS schedule [9]
Construction period (spending schedule)	3 years (8% Y1, 60% Y2, 32% Y3)
Plant salvage value	No value
Startup time	6 months
Revenue and costs during startup	Revenue = 50% of normal Variable costs = 75% of normal Fixed costs = 100% of normal
Onstream percentage after startup	90% (7,884 operating hours per year)

[a] Modified accelerated cost recovery system

***Reference:** https://www.nrel.gov/docs/fy21osti/80291.pdf; **GGE:** gallon gasoline equivalent

CFP Oil Oxygen Contents →	17%	20%	22%
Feedstock cost* ($/dry US ton)	67	67	67
Capital investment total (million $)[1]	707	728	740
Chemical coproducts	No	No	No
Electricity credit (cents/GGE)	78	57	45
MFSP[2,3] ($/GGE)	6.1-7.5	5.7-6.9	5.3-6.5
GHG Reduction over gasoline (%)	84	78	75

[1] Capital and operating costs based on the *ex situ* case in the 2015 design report (https://www.nrel.gov/docs/fy15osti/62455.pdf). Current model at lower pressure than 2015 report, leading to larger equipment sizes and higher capital costs for CFP equipment. Plant size is 2000 dry metric tonnes per day of woody feedstock.

[2] Model yields considered hydrotreated products heavier than diesel and other losses during product distillation as fuel products because the heavy ends from distillation are hydrogenated and stabilized, and can likely be used as marine fuel

[3] CFP catalyst replenishment is based on values in the 2015 design report (based on typical FCC values). The reactor heat balance is used to determine the flow rate. With a less active catalyst (reflected by different biomass to catalyst ratios in our experiments), cheaper catalyst diluents can allow CFP catalyst cost reduction.