

DOE Bioenergy Technologies Office (BETO) 2019 Project Peer Review

WBS 2.1.0.302 Thermochemical Platform Analysis – NREL

Session: Catalytic Upgrading Date: March 5, 2019

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BETO: Bioenergy Technologies Office **CFP:** Catalytic Fast Pyrolysis **DME:** Di-Methyl Ether **HOG:** High-Octane Gasoline **LCA:** Life-Cycle Analysis **MFSP:** Minimum Fuel Selling Price **MYP:** Multi-Year Plan (BETO) **SOT:** State of Technology **TEA:** Techno-Economic Analysis

Overview and Approach

Provide process design and techno-economic analysis (TEA) for thermal-catalytic conversion processes to inform and guide NREL/BETO R&D priorities

- Benchmark research goals through detailed models
- Track advancements in the State of Technology (SOT) and sustainability metrics based on experimental data
- Constant research feedback to and from TEA
- Build predictive TEA models

Quad Chart Overview – NREL TC Platform Analysis

Timeline (*current merit review cycle***)**

Budget (WBS 2.1.0.302):

†TEA: Techno-Economic Analysis, ǂLCA: Life-Cycle Assessment

Key Barriers Addressed:

Ct-F: Yield from catalytic processes ADO-A: Process integration

Objective:

To inform and guide R&D priorities for thermal and catalytic conversion processes through process-design-based TEA† and LCA^ǂ.

Partners:

- NREL & ChemCatBio (expt. & research)
- PNNL (TEA/sustainability/hydrotreating)
- Idaho National Lab & FCIC (feedstock)
- Argonne National Lab (LCA)
- DWH Consulting (modeling / capital costs)
- NIST (phase equilibrium modeling)
- Consortium for Computational Physics and Chemistry (reactor modeling)
- Johnson Matthey (catalyst technologies)
- Petrobras (petroleum refiner) via CRADA

Project Overview – Core Research & Supporting Work

Collaboration with Catalyst R&D, Experimental Data, & Catalyst Cost

> ChemCatBio & NREL Researchers, Johnson Matthey

Model Prediction of Fuel Quality & Experimental Data

> **Collaboration with** NREL Biomass Researchers and Fuels Group

Core Research Areas (Catalyst Development Driven)

Emerging Technology Options

(e.g. Co-processing, $CO₂$ upgrading)

Collaboration with Idaho National Laboratory Sustainability & Life-Cycle Analysis

Collaboration with Argonne National Laboratory

Consortium for Computational Physics and Chemistry

Technical Approach

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**

• **Financial and Feedstock Assumptions:** Consistent with BETO guidelines & related feedstock research

Example of Interaction with Research to Reduce CFP MFSP from FY17 to FY18

TEA-Identified Cost Drivers

- Pt loading
- Online/regeneration time

- Lower Pt loading
- Shorter regeneration time

Technical Progress and Accomplishments

Fixed Bed *Ex Situ* CFP Conceptual Process

Details at: <https://www.nrel.gov/docs/fy15osti/62455.pdf> and<https://www.nrel.gov/docs/fy19osti/71954.pdf>

CFP Technology Options

- Lower capital investment
- Operating conditions tied to fast pyrolysis
- Catalyst mixed with biomass, char, and ash
- Higher catalyst replacement rates
- Operating conditions can differ from fast pyrolysis
- Biomass, ash, and char are reduced or removed; more benign environment for catalyst
- Higher capital investment
- Lower catalyst replacement rates
- More diverse catalysts are feasible
- Access to greater catalytic chemistry
- Long catalyst lifetimes required
- Hot gas filter required
-

Hybrids of all or some of these systems are also possible

Timeline of CFP Technology Development Guided by TEA

Joshua A. Schaidle[®]

PNNL-23823
March 2015

<https://www.nrel.gov/docs/fy15osti/62455.pdf> [https://link.springer.com/article/10.1007](https://link.springer.com/article/10.1007/s11244-015-0500-z)

Springe

/s11244-015-0500-z

2904 | Energy Environ. Scl., 2018, 11, 2904-2918

Technical Report
NREL/TP-5100-71954
Nationalist 1918

Energy Environ. Sci., 2018, 11, 2904 <https://www.nrel.gov/docs/fy19osti/71954.pdf>

CFP: Catalytic Fast Pyrolysis, **TEA:** Techno-Economic Analysis

Ex Situ Catalytic Fast Pyrolysis – Progress

TEA-Guided Modeled-Cost Reduction from \$4.90/GGE in 2016 to \$3.50/GGE in 2018

Note: All costs are presented in 2016\$. **Reference:** [https://www.nrel.gov/docs/fy19osti/71954.pdf.](https://www.nrel.gov/docs/fy19osti/71954.pdf) **SOT:** State of Technology

Ex Situ CFP – Sustainability

****Other Sustainability Metrics for Conversion Process in Additional Slides****

- Fuel transportation and net fuel combustion
- **Biorefinery conversion**
- Depot preprocessing
- Silviculture, fertilization, harvest and collection
- Petroleum gasoline
- Co-product displacement credits
- **Transportation to biorefinery**
- Fieldside preprocessing and transportation to depot
- Supply Chain

† Reference: Cai et al. Argonne National Laboratory report, ANL/ESD-18/13, 2018. **SOT:** State of Technology

Syngas to High-Octane Gasoline Conceptual Process

HOG: High-Octane Gasoline. **Details at:** <https://www.nrel.gov/docs/fy15osti/62402.pdf> and<https://www.nrel.gov/docs/fy19osti/71957.pdf>

High-Octane Gasoline vs. Traditional MTG

*relative yield from same carbon source

Syngas Conversion to High-Octane Gasoline (HOG)

Analysis to Help Expand Product Options to Jet/Diesel

Analysis of CO₂ **Utilization & Quantification of Future Opportunities**

- Benefits of **process intensification**
- Use of low-cost feedstock and **bio-gas** utilization
- Supplemental **renewable electricity and hydrogen**

References: <https://www.nrel.gov/docs/fy15osti/62402.pdf> and<https://www.nrel.gov/docs/fy19osti/71957.pdf>. **SOT:** State of Technology

Syngas to High-Octane Gasoline – Progress

TEA-Guided Modeled-Cost Reduction from \$3.99/GGE in 2016 to \$3.79/GGE in 2018

Note: All costs are presented in 2016\$. **Reference:** [https://www.nrel.gov/docs/fy19osti/71957.pdf.](https://www.nrel.gov/docs/fy19osti/71954.pdf) **SOT:** State of Technology

Syngas to High-Octane Gasoline – Sustainability

****Other Sustainability Metrics for Conversion Process in Additional Slides****

† Reference: Cai et al. Argonne National Laboratory report, ANL/ESD-18/13, 2018. **SOT:** State of Technology

Milestones and Some Other Highlights

Milestones & Publications

- o All milestones completed (see additional slides for complete list)
	- o Go/No-Go: Identify a path to <\$3.00/GGE by 2022, with potential for <\$2.50/GGE by 2030
- o Publications listed in additional slides

Support of Work Related to Catalytic Conversion

- o Biological and catalytic upgrading of CFP aqueous phase
- o Separations consortium, FCIC, Co-Optima, ChemCatBio and others

Entrained Flow Reactor Models for Pyrolysis and Gasification

- Compatible with process simulations
- Ability to include kinetics being developed by the CCPC*
- Helps understand flow and scaling assumptions for process modeling

Reference: ACS Sustainable Chem. Eng. 2017, 5, 3, 2463-2470. ***CCPC:** Consortium for Computational Physics and Chemistry

Integration of Predictive Phase Equilibrium Models from NIST

Example of Ternary Diagram for Liquid-Liquid Equilibrium in Aspen Plus using the NIST-COSMO-SAC *Fully Predictive Model*.

Previous Pub: J. Chem. Eng. Data 2017, 62, 1, 243-252

Relevance

Provide Research Specifics for Achieving < \$3.00/GGE

****Associated Technical Parameters and Sustainability Metrics in Additional Slides**** \blacksquare Feedstock **Pyrolysis and Vapor Upgrading** Pyrolysis Vapor Quench **Hydroprocessing and Separation Hydrogen Production** ■ Balance of Plant MFSP \$/GGE of Fuel Product (2016\$) \$7.00 Significant Yield Improvement Lower Pt loading & Quicker Regeneration 23.5% Carbon Efficiency \$6.25 MFSP *Ex Situ* **Catalytic Fast Pyrolysis**\$6.00 25.9% \$5.45 28.3% \$4.90 \$5.00 38.1% \$4.09 \$4.00 39.7% 40.2% 40.9% \$3.50 \$3.46 \$3.35 41.7% 42.3% \$3.03 \$2.93 \$3.00 \$2.00 $$1.00$ \$0.00 2014 2015 2016 2017 2018 2019 2020 2021 2022

MFSP: Minimum Fuel Selling Price. **SOT:** State of Technology. Reference:<https://www.nrel.gov/docs/fy19osti/71954.pdf>

SOT

SOT

SOT

SOT

- Fluidized System -

SOT

Projection Projection Projection Projection

- Fixed Bed System -

Enabling Productive Research under BETO

- **Detailed analysis for lowering costs**
- **Sensitivity analysis and options for impactful research**
- **Deliberate attention towards enabling future commercial implementation**

Relevance to Industry and Other Stakeholders

Work Towards Commercial Viability & Product Compatibility

- **Cost reduction** to enable adoption
- **Product quality improvement** (e.g. cetane and octane)
	- Analysis for quality improvement to make fuel products more attractive
- Tailor intermediates towards higher value
	- Quantify **requirements for refinery integration** of CFP oil
- **Analysis for scale-up**
	- Direct support to facilitate pilot verification
	- Model projections for commercial implementation

Direct Use of Analysis Products by Industry, Academia, & National Labs.

- Detailed **reports and journal articles** to enable related research
- Simplified *in situ* and *ex situ* CFP **TEA models made publicly available**

Related requests are received on a regular basis

Future Work

Future Goals **Develop for Future Commercial Implementation Achieve Modeled MFSP of <\$3.00/GGE by 2022, and potentially \$2.50/GGE by 2030 (in 2016\$)**

Future Milestones and Decision Points

Proposed Go/No-Go (March 2021) (**For Pilot Verification of <\$3.00/GGE in 2022**)

Use all available experimental results to assess the chances of success for demonstrating a modeled fuel cost of <\$3.00/GGE during the 2022 verification

- Identify any gaps
- Provide options for additional cost reduction (necessary if falling short of verification goals)

Some Longer Term Work

Refinery integration of CFP streams:

- TEA for most promising options
- Quality & CFP processing requirements
- Identify metrics for success

Development of **CFP co-products**:

- TEA for identified co-products
- Identify selectivity & separation goals

****Proposed Future Milestones and Go/No-Go included in Additional Slides****

(proposed milestones beyond FY19 will be subject to merit review)

Some Specific Enablers for TEA

Chemistry-Based TEA Modeling for **Conversion Technologies** and **Refinery Integration** of CFP Fuels

Integrate experimental chemistry and related models into TEA:

- Effective feedback for catalyst development goals
- Quantify refinery co-processing requirements for integration

Models used are from literature

Implement integrated process model tracking of key fuel quality attributes with experimental speciation. Aim for predictive capability of fuel properties

Identify synergistic use of multiple technologies for more effective biorefineries

Summary

Summary

- **Overview and Approach:**
	- **State-of-the art process modeling** for TEA (includes predictive capabilities)
	- Advancements via **management plan for research** and **impactful feedback**
	- Key **success factors**: **Impactful research & future commercial implementation**
- **Technical Progress and Accomplishments** *(all milestones were met)*
	- Significant **TEA-guided advancements** for CFP **effective research options**
	- Additional **product options** analyzed for **jet/diesel** from syngas
		- Analysis of **process intensification**, utilization of **CO₂, biogas, renewable H₂ & electricity**
- **Relevance**
	- **Directly enables** BETO goal of **<\$3.00/GGE** by 2022
	- Analysis **feedback and options** used **for effective research**
	- **Commercial relevance:** Cost reduction, product compatibility, scale-up
	- Detailed **analysis products**, including **example models externally available**
- **Future Work** *(proposed future milestones & go/no-go in additional slides)*
	- **TEA for continued cost reduction** for CFP and syngas pathways
	- **Go/No-Go** for success of the <\$3.00/GGE verification

Acknowledgements

DOE BETO for funding and support

NREL (includes subcontracts) o Connor Nash

- o Zia Abdullah
- o Gregg Beckham
- o Mary Biddy
- o Adam Bratis
- o Daniel Carpenter
- o Earl Christensen
- o Abhijit Dutta
- o Chaiwat Engtrakul
- Carrie Farberow
- Jack Ferrell
- Gina Fioroni
- o Tom Foust
- o Jesse Hensley
- David Humbird
- o Kristina Iisa
- Chris Kinchin
- o Kim Magrini
- o Bob McCormick
- o Calvin Mukarakate
- o Mark Nimlos
- o Dan Ruddy
- o Josh Schaidle
- o Avantika Singh
- o Michael Talmadge
- o Eric Tan
- o Suphat Watanasiri
- o Matt Wiatrowski
- o Nolan Wilson
- o Erick White
- o Thermochemical research team
- o Biorefinery analysis team

PNNL

- o Corinne Drennan
- o Susanne B. Jones
- o Aye Meyer
- o Steve Phillips
- o Lesley Snowden-Swan

INL

- o Damon Hartley
- o David Thompson

ANL

o Hao Cai

NIST-TRC

- o Vladimir Diky
- o Kenneth Kroenlein
- o Chris Muzny
- o Eugene Paulechka
- **Feedstock Interface (FCIC)**

Johnson Matthey

ChemCatBio

Consortium for

- **Computational Physics and Chemistry (CCPC)**
-
- **Co-Optima**
- **Petrobras**
- **Separations Consortium**

Additional Slides for Reviewers

Additional Slides – Table of Content

Project Abstract and PI Biography

Milestones & Go/No-Go (completed and future)

Responses to 2017 Peer Review Comments

Additional Technical Content - CFP

Additional Technical Content – Syngas to HOG

NREL Thermochemical Platform Analysis (WBS 2.1.0.302)

The objective of the NREL Thermochemical Platform Analysis (WBS 2.1.0.302) project is to inform and guide R&D priorities for thermal and catalytic conversion processes by providing process design and techno-economic analysis (TEA). This is achieved through close collaboration with researchers and external experts, along with the use of both commercially-available modeling tools and the development or use of partner-developed domain-specific tools and resources, such as refinery integration, kinetic and reactor models, phase equilibrium models, and pertinent bio-products market studies.

This project is directly aligned with DOE-BETO goals; this includes the reduction of projected conversion costs for biomass derived fuels and products by enabling research advancements. TEA-guided research has helped achieve significant modeled cost reductions for the *ex situ* catalytic fast pyrolysis (CFP) pathway since the previous peer review in 2017 and we have identified specific research steps to help reduce the modeled Minimum Fuel Selling Price (MFSP) to <\$3.00/GGE by 2022. Further cost reduction through refinery integration, development of valuable co-products, and other options are being identified for future research to help reduce the modeled MFSP to \$2.50/GGE by 2030. Additional priorities anticipated in the future, such as the use of renewable electricity for liquid fuels and products, and emphasis on waste utilization are also being explored in conjunction with research on catalytic utilization of syngas and other gases. Industry-relevant parameters are given deliberate attention as part of the work done under this project to help answer questions important for future commercialization.

Abhijit Dutta, Principal Investigator

Abhijit Dutta is a senior engineer in the National Bioenergy Center (NBC) at the National Renewable Energy Laboratory (NREL). He has a Master's degree in Chemical Engineering with more than 20 years of experience in process engineering and simulator development. His expertise includes process modeling and techno-economic analysis for thermal and catalytic conversion processes. He has led the analysis work for the Thermochemical Platform Analysis (NREL) project for nearly a decade and has multiple publications based on his work at NREL. Prior to joining NREL, Dutta worked at Bloom Energy and Aspen Technology on process control and simulator development.

NREL Employee Webpage: <https://www.nrel.gov/research/abhijit-dutta.html>

Milestones (FY2018)

FY2018 Go/No-Go Summary

Identify options for cost reduction to <\$3.00/GGE by 2022 with potential for <\$2.50/GGE by 2030

*2030 projections are based on high-level estimates that will be modeled in detail in future years

All milestones (to date) completed on time

Future Milestones (Preliminary)

Responses to 2017 Peer Review Comments

Overall Impressions/Comments from Reviewers (key excerpts):

- Some complementary excerpts (selected a few): Strong project with a history of successfully providing key information; earlier work matched the results from the analysis from my similar process development work. Well-managed with clearly defined barriers and critical issues.
- Some comments with specific recommendations (paraphrased): **(i)** Use the tools to evaluate outside work and validate the tools using well understood technologies; **(ii)** include risk & outside factors that influence the values; **(iii)** large project with many aspects made it difficult for the reviewer fully understand; more examples would be helpful for reviewers; **(iv)** more dissemination of work and some of the products allowing evaluation of outside work.

PI Response to the Above Comments (with current information):

• Thank you for your helpful feedback and guidance. We will continue to be diligent in the recommended areas. Here are some responses/actions for the specific comments/recommendations: **(i)** The methods used & correctness of our economic spreadsheet tool (subject to our assumptions), have been validated by multiple organizations (including industry and academia) since we started making the tools publicly available (close to the year 2000). Our process modeling efforts include rigorous heat and energy balances in Aspen Plus, industrial data/results (for published and mature processes), and experimental data and research projections (for our research areas). While we do not have the funding or scope to extensively evaluate outside technologies, our methods make significant use of published industrial information wherever available (and an industry-standard capital cost estimation tool). We use experimental validation for our tools, whenever feasible, e.g. our predictive phase equilibrium work with NIST has an experimental validation component. We engage engineering firms for larger design report projects, with significant review by external experts (including from industry). One of the peer reviewers commented that results from our analysis matched the analysis done for similar process development done by that reviewer. **(ii)** We have the capability to include risk information, and report some of it as part of sensitivity analysis. Our base case values are used to benchmark research goals and progress (hence don't directly include risk information – this allows a clean comparison of research progress using consistent metrics). **(iii)** The project scope is now significantly streamlined, reflecting a smaller scope and associated funding reductions. This 2019 presentation includes examples. **(iv)** We made additional models publicly available since the previous peer review. Also, our major publications most often contain sufficient details for re-creating the models. Previous details available at: https://www.energy.gov/sites/prod/files/2018/02/f48/2017_peer_review_thermochemical_conversion.pdf

Publications and Presentations since 2017 Peer Review

Slide 1 of 2

- Griffin, M.B; Iisa, K.; Wang, H.; Dutta, A.; Orton, K.A.; French, R.J.; Santosa, D.M.; Wilson, N.; Christensen, E.; Nash, C.; Van Allsburg, K.M.; Baddour, F.G.; Ruddy, D.A.; Tan, E.C.D.; Cai, H.; Mukarakate, C.; Schaidle, J.A.. Driving towards cost-competitive biofuels through catalytic fast pyrolysis by rethinking catalyst selection and reactor configuration. Energy Environ. Sci., 2018. <http://dx.doi.org/10.1039/C8EE01872C>
- Dutta, A.; Iisa, K.; Mukarakate, C.; Griffin, M.; Tan, E.C.D.; Schaidle, J.; Humbird, D. et al. 2018. Ex Situ Catalytic Fast Pyrolysis of Lignocellulosic Biomass to Hydrocarbon Fuels: 2018 State of Technology and Future Research. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-71954. [https://www.nrel.gov/docs/fy19osti/71954.pdf.](https://www.nrel.gov/docs/fy19osti/71954.pdf)
- Tan, E.C.D.; Ruddy, D.; Nash, C.; Dupuis, D.; Dutta, A.; Hartley, D.; Cai, H. 2018. High-Octane Gasoline from Lignocellulosic Biomass via Syngas and Methanol/Dimethyl Ether Intermediates: 2018 State of Technology and Future Research. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-71957. [https://www.nrel.gov/docs/fy19osti/71957.pdf.](https://www.nrel.gov/docs/fy19osti/71957.pdf)
- Dunn, J.B; Biddy, M.; Jones, S.; Cai, H.; Benavides, P.T.; Markham, J.; Tao, L.; Tan, E.; Kinchin, C.; Davis, R.; Dutta, A.; Bearden, M.; Clayton, C.; Phillips, S.; Rappé, K.; Lamers, P. Environmental, economic, and scalability considerations and trends of selected fuel economy-enhancing biomass-derived blendstocks. ACS Sustainable Chem. Eng., 2018, 6 (1), pp 561–569.
- Zhang, Y.; Sahir, A.H.; Tan, E.C.D.; Talmadge, M.S.; Davis, R.; Biddy, M.J.; Tao, L. Economic and Environmental Potentials for Natural Gas to Enhance Biomass-to-Liquid Fuels Technologies. Green Chem., 2018,20, 5358-5373.
- Iisa, K.; Robichaud, D.J.; Watson, M.J.; ten Dam, J.; Dutta, A.; Mukarakate, C.; Kim, S.; Nimlos, M.R.; Baldwin, R.M. Improving biomass pyrolysis economics by integrating vapor and liquid phase upgrading. First published Nov 24, 2017. Green Chemistry. DOI: 10.1039/c7gc02947k.
- Iisa, K.; French, R.J.; Orton, K.A.; Dutta, A.; Schaidle, J.A. Production of low-oxygen bio-oil via ex situ catalytic fast pyrolysis and hydrotreating. Fuel 207 (2017) 413–422.

Publications and Presentations since 2017 Peer Review

Slide 2 of 2

- Tan, E.C.D.; Biddy, M. An Integrated Sustainability Evaluation of Indirect Liquefaction of Biomass to Liquid Fuels. 7th International Congress on Sustainability Science & Engineering (ICOSSE '18: Industry, Innovation and Sustainability), Cincinnati, OH, August 12-15, 2018. **(Presentation)**
- Tan, E.C.D.; Cai, H.; Talmadge, M. Relative Sustainability of Natural Gas Assisted High-Octane Gasoline Blendstock Production from Biomass. 2017 AIChE Annual Meeting, Minneapolis, MN, October 29–November 3, 2017. **(Presentation)**
- Ruddy, D.A.; Nash, C.; Hensley, J.; Schaidle, J.; Farberow, C.; Cheah, S.; Tan, E.; Talmadge, M. Isobutane Activation over a Cu/BEA Catalyst and Re-Incorporation into the Chain-Growth Cycle of Dimethyl Ether Homologation. 25th North American Meeting of the Catalysis Society, Denver, CO, June 4-9, 2017. **(Presentation)**

Additional content for conversion pathways:

- Catalytic Fast Pyrolysis (CFP)
- High-Octane Gasoline (HOG)

Catalytic Fast Pyrolysis – SOT and Projections

Catalytic Fast Pyrolysis– Tables from MYP (1)

Catalytic Fast Pyrolysis– Tables from MYP (2)

Catalytic Fast Pyrolysis– Tables from MYP (3)

^a Conceptual design results.

^b Gallon gasoline equivalent on a lower heating value basis.

c A negligible stream was maintained in the model to allow natural gas use if necessary.

d 2030 projections are based on high-level estimates and will be modeled in detail in future years. It is proposed that hydroprocessing will occur at a petroleum refinery with coprocessing of the catalytic fast pyrolysis oils using existing capital. Capital for hydrogen production is included, while natural gas feed for hydrogen production is not included because credit is not taken for an equivalent amount of fuel gas from the CFP biorefinery. Coproduct credit is based on a preliminary estimate of diverting 20% CFP oil to produce coproducts

Ex Situ CFP – Sustainability Metrics Summary

>60% GHG reduction over petroleum derived gasoline per ANL analysis†

Note: Metrics shown apply to conversion process only

† Reference: Cai et al. Argonne National Laboratory report, ANL/ESD-18/13, 2018.

High-Octane Gasoline – SOT and Projections

Details included in tables on following slides

High-Octane Gasoline – Tables from MYP (1)

High-Octane Gasoline – Tables from MYP (2)

High-Octane Gasoline – Tables from MYP (3)

High-Octane Gasoline – Tables from MYP (4)

*Conceptual design results.

HOG – Sustainability Metrics Summary

>60% GHG reduction over petroleum derived gasoline per ANL analysis†

Note: Metrics shown apply to conversion process only. *****Includes LPG product **†Reference:** Cai et al. Argonne National Laboratory report, ANL/ESD-18/13, 2018.

HOG Pathway Related Information

Details at: <https://www.nrel.gov/docs/fy15osti/62402.pdf>

Margin for Premium Gasoline

HOG Pathway Sensitivity: Jet Fuel Analysis

C₄-C₈ olefin coupling produces a C₈-C₂₀ distribution of HCs, **with >90% being suitable as a jet fuel blendstock**

M. Behl, et al., *Energy & Fuels* 29 **2015** 6078, NREL Milestone Report Dec 2015.