



High-Octane Gasoline from Lignocellulosic Biomass via Syngas and Methanol/Dimethyl Ether Intermediates: 2020 State of Technology

Kylee Harris,¹ Daniel Ruddy,¹ Connor Nash,¹ Abhijit Dutta,¹ Daniel Dupuis,¹ Eric Tan,¹ Damon Hartley,² and Hao Cai³

1 National Renewable Energy Laboratory

2 Idaho National Laboratory

3 Argonne National Laboratory

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Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-79986
July 2021



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Suggested Citation

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>.

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National Renewable Energy Laboratory
15013 Denver West Parkway
Golden, CO 80401
303-275-3000 • www.nrel.gov

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This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Bioenergy Technologies Office. The views expressed herein do not necessarily represent the views of the DOE or the U.S. Government.

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Acknowledgments

The authors wish to thank the following contributors from the National Renewable Energy Laboratory (NREL): Jesse Hensley for some preliminary experimental design discussion; Josh Schaidle for reviewing this report and providing valuable comments; and Michael Deneen and Kathy Cisar for communications support.

Nomenclature

ANL	Argonne National Laboratory
BETO	Bioenergy Technologies Office
Btu	British thermal unit
DME	dimethyl ether
FY	fiscal year
GGE	gallon of gasoline equivalent
HHV	higher heating value
HMB	hexamethylbenzene
HOG	high-octane gasoline
iC4	isobutane
IDL	indirect liquefaction
INL	Idaho National Laboratory
IRR	internal rate of return
LHV	lower heating value
LPG	liquid petroleum gas
MFSP	minimum fuel selling price
MM	million
NREL	National Renewable Energy Laboratory
SOT	state of technology
TEA	techno-economic analysis

Executive Summary

This report was developed as part of the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Bioenergy Technologies Office's (BETO's) efforts to enable the development of technologies for the production of infrastructure-compatible, cost-competitive liquid hydrocarbon fuels from lignocellulosic biomass feedstocks. This report details the 2020 state of technology (SOT) assessment of the production of high-octane gasoline (HOG) via indirect liquefaction (IDL) based on the assumption of similar reactor performance in a scaled-up conceptual design model as in our bench-scale experimental system.

The conceptual design produces HOG via the sequential conversion of lignocellulosic biomass to syngas, syngas-to-methanol, methanol-to-dimethyl ether (DME), and ultimately DME-to-HOG. In this analysis, we focused primarily on the advancement of downstream homologation of DME to branched hydrocarbons. The key experimental results and associated technical accomplishments achieved in this fiscal year (FY) 2020 include reduced aromatics formation in the DME-to-HOG step, reduced uncertainty relating to the reincorporation of recycled light hydrocarbons, and process optimization within the model. Experimental data was collected for this 2020 assessment; this included a range of isobutane-to-DME recycle ratios to enable techno-economic analysis (TEA) to evaluate the effect on modeled product yields and associated costs. Each data set was an average from at least six analysis points from at least two repeats at the same experimental inputs/conditions. Among the multiple experimental data sets, results with an isobutane-to-DME ratio of 1.2 provided the highest yields; this was chosen as the base case for the 2020 SOT and is presented in Table ES-1. The results show that the FY 2020 cost target of \$3.49 per gallon of gasoline equivalent (GGE) was achieved. Specifically, this case shows that a modeled minimum fuel selling price (MFSP) of \$3.45/GGE can be achieved by including experimental performance in the updated model. Considering uncertainty in our analysis of key experimental variables, the MFSP has a range of \$3.38-3.56/GGE. Future research is required to further reduce aromatics selectivity from the current value of 3.3% to the 2022 target of 0.5%, and to continue to improve the light hydrocarbon re-incorporation efficiency. Both of these will serve to increase C5+ carbon selectivity and further improve cost and carbon efficiency.

This 2020 SOT update also included a rebuild of the Aspen Plus model used for previous SOT assessments. The rebuild was necessary because the model needed to be better equipped to incorporate research information and changes in research strategy since the initial version created in 2014; however, the underlying conceptual design and capital estimations remained largely the same. The model updates began by streamlining the Aspen Plus model to significantly shorten convergence times, while maintaining the same overall process design. Other changes in the TEA model led to more optimal recycle, heat integration, and separations. For example, the liquid petroleum gas (LPG) coproduct was eliminated to allow a higher HOG product yield by re-incorporating some isobutane in the DME conversion step, and routing excess isobutane and LPG range products to the reformer to produce more syngas. Additionally, higher pressure in the DME-to-HOG conversion step was adopted to facilitate lower separation costs and a smaller reactor volume (associated increases in compression costs were included). The inclusion of multiple isobutane-to-DME ratio experiments eliminated previous yield assumptions based on extrapolation of the isobutane-to-DME recycle ratio in this FY 2020 model (extrapolations were used in the FY 2019 model). Finally, the new model improved integration, with reduced waste and the reuse of existing process streams. Note again that we did not change base equipment

costs or unit operating costs, or otherwise alter any fundamental assumptions that could change the cost basis in the updated model. A summary of key metrics is presented below (more details are included in the main body of the report). Detailed cost breakdowns are included in Table ES-2 (2020 SOT) and Table ES-3 (2022 projection). Technical advancements necessary for future improvements are presented in the Appendix.

Table ES-1. Performance Metrics for the 2019 SOT, 2020 SOT, and 2022 Projection

Performance Metrics	2019 SOT^a	2020 SOT	2022 Projection
DME Conversion (%)	44.7 ^b	43.4 ^b	40 ^b
C5+ C-Selectivity (%)	73.6 ^c	72.07 ^c	86.7 ^c
Aromatics C-Selectivity (%)	5.8	3.3	0.5
HOG Hydrocarbon Productivity (kg/kg-catalyst/h)	0.07	0.09	0.1
HOG Product Yield (GGE/dry U.S. ton)	49	51.4	54.7
LPG Coproduct (GGE/dry U.S. ton)	5.6	—	—
MFSP (\$/GGE; 2016\$)	3.53	3.45	3.30
Fuel Synthesis and Separation Cost^d (¢/GGE; 2016\$)	49	45	48

^a As reported in FY 2020; there were some updates to the MFSP due to upgrades to a new version of Aspen Plus; we continue to use the published numbers (using a previous version of Aspen Plus). Note that the 2019 SOT included some extrapolated yields, which is no longer the case in the FY 2020 SOT.

^b Single-pass conversion

^c Overall selectivity

^d 2020 SOT values are reported as a sum the hydrocarbon synthesis and hydrocarbon product separation costs as reported in Figure A-1. 2019 SOT and 2022 projection values are reported in total in the hydrocarbon synthesis section (Figure A-1).

Table ES-2. Economic Summary for 2020 SOT

Process Engineering Analysis for High Octane Gasoline via Indirect Gasification and Methanol Intermediate : 2020 SOT

2,000 Dry Metric Tonnes Biomass per Day

Indirect Gasifier, Tar Reformer, Sulfur Removal, Methanol Synthesis, Hydrocarbon Synthesis on Cu-Beta-Zeolite Catalyst, Fuel Purification, Steam-Power Cycle

All Values in 2016 US\$

Minimum Fuel Selling Price		\$3.45 per GGE	
(MFSP, Gasoline-Equivalent Basis)			
Feedstock & In-Plant Handling Costs		1.230 per GGE	
Operating Costs & Credits		0.860 per GGE	
Capital Charges & Taxes		1.358 per GGE	
Fuel Production at Operating Capacity		37.22 MM GGE per Year	
Fuel Product Yield		51.39 GGE per Dry US Ton Feedstock	
LPG Production at Operating Capacity		0.0 MM GGE per Year	
LPG Product Yield		0.0 GGE per Dry US Ton Feedstock	
Delivered Feedstock Cost		\$63.23 per Dry US Ton	
Capital Costs		Annual Operating Costs	
Area A100: Feed Handling & Preparation	\$200,000	Feedstock	\$45,800,000
Area A200: Gasification	\$47,400,000	Natural Gas	\$0
Area A300: Syngas Cleanup and Compression	\$69,300,000	Catalysts	\$9,100,000
Area A400: Acid Gas Removal and Hydrogen Recovery	\$16,600,000	Olivine	\$600,000
Area A400SM: Syngas Conversion to MeOH (& Separations)	\$18,000,000	Other Raw Matl. Costs	\$1,500,000
Area A400MD: MeOH Conversion to DME (& Separations)	\$4,300,000	Waste Disposal	\$1,000,000
Area A400DH: DME Conversion to HOG	\$15,300,000	Electricity Transfer Charge	\$0
Area A400HCND: HOG Separations	\$9,900,000	Electricity	\$0
Area A600: Steam System & Power Generation	\$43,600,000	Fixed Costs	\$19,900,000
Area A700: Cooling Water & Other Utilities	\$7,600,000	Coproduct credits (including electricity)	\$0
Area A800: WWT & H2O Management	\$1,700,000	Capital Depreciation	\$12,900,000
Total Installed Equipment Cost (TIC)	\$233,900,000	Average Income Tax	\$3,600,000
 		Average Return on Investment	\$34,100,000
ISBL (Areas A100 to A400)	\$171,100,000	 	
OSBL (Areas A600 to A700)	\$61,100,000	Operating Costs per Product	(¢/MMBtu) (¢/GGE)
 		Feedstock	1059.8 123.0
Other Direct Costs	\$7,200,000	Natural Gas	0.0 0.0
(% of ISBL)	4.0%	Catalysts	210.0 24.4
 		Olivine	13.1 1.5
Total Direct Costs (TDC)	\$241,300,000	Other Raw Materials	35.1 4.1
 		Waste Disposal	23.0 2.7
Indirect Costs	\$144,800,000	Electricity Transfer	0.0 0.0
(% of TDC)	60.0%	Electricity	0.0 0.0
 		Fixed Costs	460.2 53.4
Land Purchase Cost	1,600,000	Coproduct credits	-0.5 -0.1
Working Capital	19,300,000	Capital Depreciation	298.6 34.7
 		Average Income Tax	82.9 9.6
Total Capital Investment (TCI)	407,100,000	Average Return on Investment	788.7 91.6
 		Total (Plant Gate Price)	2970.9 344.90
Installed Equipment Cost per Annual Gallon	\$6.28	 	
Total Capital Investment per Annual Gallon	\$10.94	Power Balance	(KW) (hp)
 		Total Plant Power Consumption (KW)	42,788 57,380
Debt Financing (% of Investment)	60.0%	Power Generated Onsite (KW)	42,791 57,384
Loan Interest Rate	8.0%	Power Imported from Grid (KW)	0 0
Loan Term (years)	10.0	Power Exported to Grid (KW)	3 5
Equity Financing (% of Investment)	40.0%	Power Generation	(KW) (hp)
Internal Rate of Return (After-Tax)	10.0%	Steam Turbine Generators	41,014 55,001
 		Process Gas Turboexpander(s)	1,777 2,383
Plant Operating Hours per year	7,884	 	
On-Stream Percentage	90.0%	Sustainability Metrics	
 		Plant Electricity Consumption (KWh/ GGE)	9.1
Process Efficiency		Gasification & Reforming Steam (lb / GGE)	23.3
Gasifier Efficiency - HHV %	78.5	Water Consumption (Gal Water / GGE)	3.28
Gasifier Efficiency - LHV %	78.0	Carbon Conversion Efficiency (C in Fuel/C in Feedstock)	26.11%
Efficiency to Gasoline - HHV %	37.9	 	
Efficiency to Gasoline - LHV %	37.6	Feedstock Rate and Cost	
Overall Plant Efficiency - HHV %	37.9	Feed Rate	Dry Tonnes / Day 2,000
Overall Plant Efficiency - LHV %	37.6		Dry US Tons / Day 2,205
 		Feedstock Cost	\$ / Dry Ton \$63.23
Excel File: HOG2020-V117b_rev6_sens.xlsm			\$ / Moisture & Ash Free Ton \$64.36

Table ES-3. Economic Summary for 2022 Projection

Process Engineering Analysis for High Octane Gasoline via Indirect Gasification and Methanol Intermediate

2,000 Dry Metric Tonnes Biomass per Day

Indirect Gasifier, Tar Reformer, Sulfur Removal, Methanol Synthesis, Hydrocarbon Synthesis on Cu-Beta-Zeolite Catalyst, Fuel Purification, Steam-Power Cycle
All Values in 2016 US\$

Minimum Fuel Selling Price	
(MFSP, Gasoline-Equivalent Basis)	\$3.30 per GGE
Contributions: Feedstock Costs	1.108 per GGE
Operating Costs & Credits	0.655 per GGE
Capital Charges & Taxes	1.538 per GGE
Fuel Production at Operating Capacity	39.59 MM GGE per Year
Fuel Product Yield	54.66 GGE per Dry US Ton Feedstock
LPG Production at Operating Capacity	0.0 MM GGE per Year
LPG Product Yield	0.0 GGE per Dry US Ton Feedstock
Delivered Feedstock Cost	\$60.54 per Dry US Ton

<u>Capital Costs</u>		<u>Annual Operating Costs</u>		
Feed Handling & Drying	\$200,000	Feedstock		\$43,800,000
Gasification	\$44,600,000	Natural Gas		\$0
Gas Cleanup	\$52,800,000	Catalysts		\$11,700,000
Methanol Synthesis	\$33,700,000	Olivine		\$600,000
Methanol Conditioning	\$2,300,000	Other Raw Matl. Costs		\$1,500,000
DME & Hydrocarbons Conversion	\$47,300,000	Waste Disposal		\$1,600,000
Gasoline Separations	\$5,000,000	Electricity Transfer Charge		\$0
Steam System & Power Generation	\$34,700,000	Electricity		\$0
Cooling Water & Other Utilities	\$7,200,000	Fixed Costs		\$19,500,000
Total Installed Equipment Cost (TIC)	\$227,800,000	Coproduct credits		\$0
		Capital Depreciation		\$12,500,000
ISBL (Areas A100 to A500, A1400, A1500)	\$185,900,000	Average Income Tax		\$3,900,000
OSBL (Areas A600, A700)	\$41,900,000	Average Return on Investment		\$44,500,000
Other Direct Costs	7,400,000	<u>Operating Costs per Product</u>		
(% of ISBL)	4.0%		(c/MMBtu)	(c/GGE)
		Feedstock	954.0	110.8
Total Direct Costs (TDC)	235,265,659	Natural Gas	0.0	0.0
		Catalysts	59.6	6.9
Indirect Costs	141,200,000	Olivine	12.1	1.4
(% of TDC)	60.0%	Other Raw Materials	33.1	3.8
		Waste Disposal	34.7	4.0
Land Purchase Cost	1,600,000	Electricity Transfer	0.0	0.0
Working Capital	18,800,000	Electricity	0.0	0.0
		Fixed Costs	424.8	49.3
Total Capital Investment (TCI)	396,900,000	Coproduct credits	0.0	0.0
		Capital Depreciation	272.0	31.6
Installed Equipment Cost per Annual Gallon	\$5.62	Average Income Tax	84.4	9.8
Total Capital Investment per Annual Gallon	\$9.79	Average Return on Investment	968.6	112.4
		Total (Plant Gate Price)	2843.3	330.1
Debt Financing (% of Investment)	60.0%	<u>Power Balance</u>		
Loan Interest Rate	8.0%		(KW)	(hp)
Loan Term (years)	10.0	Total Plant Power Consumption (KW)	36,084	48,389
		Power Generated Onsite (KW)	36,049	48,342
Equity Financing (% of Investment)	40.0%	Power Imported from Grid (KW)	35	47
Internal Rate of Return (After-Tax)	10.0%	Power Exported to Grid (KW)	0	0
Plant Operating Hours per year	7,884	<u>Power Generation</u>		
On-Stream Percentage	90.0%		(KW)	(hp)
		Steam Turbine Generators	34,419	46,157
		Process Gas Turboexpander(s)	1,630	2,186
<u>Process Efficiency</u>		<u>Sustainability Metrics</u>		
Gasifier Efficiency - HHV %	72.3	Plant Electricity Consumption (KWh/ GGE)		7.2
Gasifier Efficiency - LHV %	71.9	Gasification & Reforming Steam (lb / GGE)		20.5
Efficiency to Gasoline - HHV %	40.7	Water Consumption (Gal Water / GGE)		2.8
Efficiency to Gasoline - LHV %	40.4	Carbon Conversion Efficiency (C in Fuel/C in Feedstock)		27.95%
Overall Plant Efficiency - HHV %	40.7			
Overall Plant Efficiency - LHV %	40.4	<u>Feedstock Rate and Cost</u>		
		Feed Rate	Dry Tonnes / Day	2,000
			Dry US Tons / Day	2,205
		Feedstock Cost	\$ / Dry Ton	\$60.54
			\$ / Moisture & Ash Free Ton	\$62.41

Excel File: 2022 Design FR Rev5a_2 KH (Feedstock Cost).xslm

Sensitivity studies were conducted to identify cost drivers and to understand how experimental performance metrics will impact overall cost in future research efforts. In a single-point sensitivity analysis around the base case, it was determined that increasing single-pass DME conversion from 43.4% to 52.1% reduced the MFSP from \$3.45/GGE to \$3.41/GGE, while a decrease of the same magnitude to 34.7% increased the MFSP to \$3.51/GGE. Another key process parameter is the productivity of the hydrocarbon synthesis catalyst. A 20% increase from the base case productivity of 0.09 g/g-cat/h yielded an improved MFSP of \$3.42/GGE while a 20% decrease resulted in an MFSP of \$3.49/GGE. To set a range on the MFSP based on uncertainty in key process parameters, these cases were combined to give an overall MFSP range of \$3.38-\$3.56/GGE. Sensitivities were also included giving consideration to available federal carbon tax credits. This process could fall under the 45Q carbon capture tax credit, in which eligible facilities can receive up to a \$50/ton CO₂ captured incentive depending on the end use of carbon. Because an acid gas removal step is already incorporated into the process design, yielding a nearly pure CO₂ stream, it is feasible that this carbon could be sequestered or used for advanced CO₂ to fuels and chemicals technologies. A sensitivity study performed in which credits were applied at increments of \$10/ton CO₂ captured up to \$40/ton, as shown in Figure ES-1. An upper limit credit value of \$40/ton, rather than \$50/ton, was selected to account for additional CO₂ purification, compression, and transportation costs which are not yet factored into the model. The lower ranges were included to factor in other potential uncertainties of the actual credit value. Whereas the 2020 SOT (\$3.45/GGE) achieves the 2020 target of \$3.49/GGE without any CO₂ credit, inclusion of the 45Q credits at the \$20/ton CO₂ level helps achieve the 2022 target of \$3.30/GGE. Taking the full \$40/ton credit reduces the MFSP to \$3.12/GGE. Note that the life cycle analysis does not reflect the potential sequestration or reuse of the pure CO₂ stream; the greenhouse gas impact of the process can be further improved if accounting for potential CO₂ sequestration.

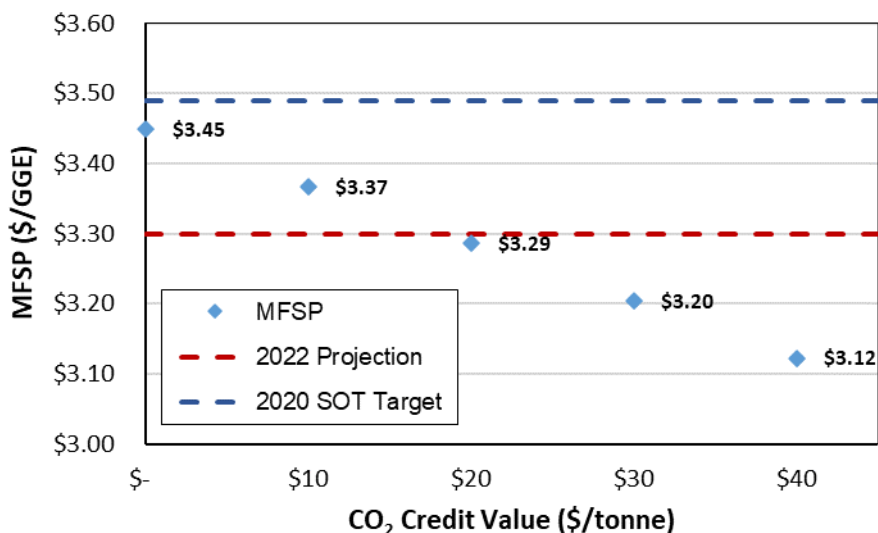


Figure ES-1. MFSP as a function of CO₂ credit value

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1 Introduction

This report is a 2020 update for the state of technology (SOT) and research improvements for the indirect liquefaction (IDL) of woody biomass to high-octane gasoline (HOG) pathway. Presented in this report are the experimental metrics marking improvements using the National Renewable Energy Laboratory's (NREL's) Cu/BEA catalyst. These metrics were used in models to generate the accompanying techno-economic analysis (TEA) and sustainability assessment for a scaled-up conceptual process. The 2020 results are compared to both 2019 SOT values and the 2022 projection case for reference. The 2020 SOT model is based on the underlying principles and process design outlined in NREL's 2015 design report [1]. This report will focus on progress since the 2019 update [2].

Research efforts since 2019 resulted in Cu/BEA catalyst improvements that led to better dimethyl ether (DME)-to-HOG reactor performance. The Cu/BEA catalyst's key performance metrics include single-pass DME conversion, selectivity to gasoline-range products (C5+), productivity, selectivity to aromatics and coke precursors, and isobutane (iC4) recycle efficiency. Key findings from previous years indicated that the recycle and reactivation of iC4 has favorable effects on HOG yield and minimum fuel selling price (MFSP); thus, performance of the HOG synthesis reactor with co-fed iC4 is an important focus area noted in this report. For this 2020 SOT, the experimental performance metrics were updated and supplemented to include multiple data points covering various iC4-to-DME ratios in the reactor feed.

In addition to experimental progress, updates were made to the Aspen Plus process model to allow more flexibility and quicker computational times. The updated model maintained the same underlying capital and operating cost bases as previous models. The subsequent sections summarize feedstock information from Idaho National Laboratory (INL), experimental development and techno-economic analysis from NREL, and conversion process sustainability assessment from Argonne National Laboratory (ANL).

2 Process Description and Assumptions

A simplified process flow diagram of the 2020 SOT model is shown in Figure 1. The overall process design features four major processing steps: (1) indirect gasification of biomass to clean syngas, (2) catalytic conversion of syngas to methanol, (3) methanol dehydration to DME, and (4) DME homologation to branched hydrocarbons. Detailed process design information for the conversion of biomass to clean syngas is available from previous Bioenergy Technologies Office (BETO)-funded reports [1–3]. Syngas to methanol (step 2) and methanol dehydration to DME (step 3) are based on commercially operated processes. The bulk of the advancements and process modifications were related to developments in the conversion of DME to branched hydrocarbons. Advancements included increased single-pass DME conversion, increased C5+ product selectivity, and low aromatics production. The details of these changes are outlined later in this report.

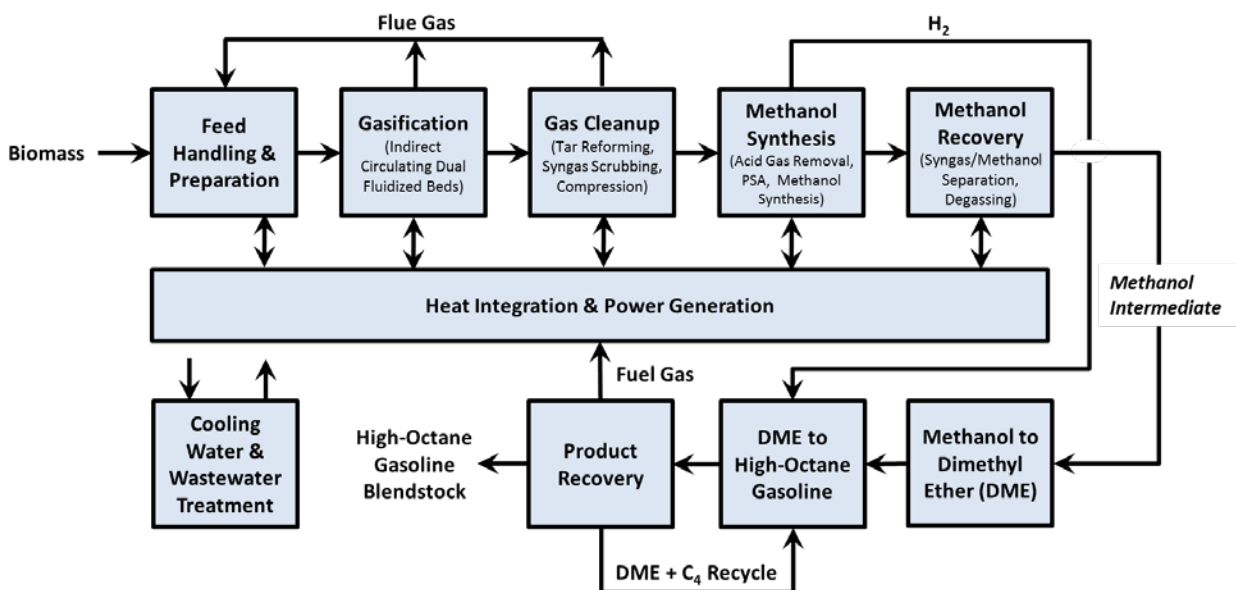


Figure 1. Process flow diagram for the production of high-octane gasoline blendstock via syngas conversion pathway and methanol/dimethyl ether intermediates

PSA = pressure swing adsorption

3 Feedstock Specifications and Costs

The 2020 IDL SOT feedstock composition and cost information used in this analysis was provided by INL and is described in detail in INL's *Woody Feedstocks 2020 State of Technology Report* [4]. Overall, feedstock specifications remained consistent with those reported in the 2019 IDL SOT report [2]. The delivered feedstock cost was calculated by INL and set at \$63.23/dry U.S. ton. The woody feedstock is a 50% clean pine, 50% forest residue blend with an ash content of 1.75 wt % and a delivered moisture content of 30 wt %. A detailed elemental breakdown is shown in Table 1. To meet the proper feed specifications for the gasifier, the feedstock is dried from a moisture content of 30 wt % to a moisture content of 10 wt % using waste heat from the biorefinery.

Table 1. Woody Feedstock Specifications Used in the 2020 SOT Process Model

Component	Weight % (Dry Basis)
Carbon	50.45
Hydrogen	5.99
Nitrogen	0.17
Chlorine	0.00
Sulfur	0.09
Oxygen	41.55
Ash	1.75
Heating Value ^a (Btu/lb)	8,533 HHV ^b 7,933 LHV ^c

^a Calculated using the Aspen Plus Boie correlation

^b Higher heating value

^c Lower heating value

4 Financial Assumptions for Techno-Economic Analysis

The TEA reported here uses n^{th} -plant economic assumptions. The key assumption associated with n^{th} -plant economics is that a successful industry has been established with many operating plants using similar process technologies. The TEA model encompasses a process model and an economic model. For a given set of conversion parameters, the process model solves mass and energy balances for each unit operation. These data are used to size and cost process equipment and compute raw material and other operating costs. The capital and operating costs are then used for a discounted cash flow rate of return analysis. An MFSP required to obtain a net present value of zero for a 10% internal rate of return (IRR) on the equity (also known as discount rate) is determined. Further discussion about the TEA model is available in the previous design report [1]. A summary of the assumptions applied in this report is listed in Table 2.

Table 2. Summary of n^{th} -Plant Assumptions for Techno-Economic Analysis

Description of Assumption	Assumed Value
Cost year	2016 U.S. dollars
IRR 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 (excluding land purchase cost)
Depreciation schedule	7-year MACRS schedule ^a
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
On-stream percentage after startup	90% (7,884 operating hours per year)

^a Modified accelerated cost recovery system

5 2020 SOT

5.1 Experiment and Results

The current research efforts focus on the DME-to-HOG step in which DME undergoes homologation to primarily form branched paraffin hydrocarbons. The direct homologation of DME into alkanes and water is hydrogen-deficient, resulting in the formation of unsaturated alkylated aromatic residues, which reduce yield and can contribute to catalyst deactivation. NREL researchers have overcome this challenge by developing a Cu-modified H-BEA catalyst (Cu/BEA) that is able to incorporate hydrogen from gas-phase H₂ co-fed with DME into the desired branched alkane products while maintaining the high C₄ and C₇ carbon selectivity of the parent H-BEA [5]. The Cu/BEA catalyst is a multifunctional catalyst. It activates co-fed hydrogen and incorporates it into the hydrocarbon products, increasing paraffin selectivity and decreasing aromatics selectivity.

Additionally, the Cu/BEA catalyst exhibits C₄ reactivation capability, exemplified experimentally using isobutane. C₄ hydrocarbons can be recycled back to the DME-to-hydrocarbons reactor, significantly increasing the overall C₅₊ hydrocarbons product selectivity. Noticeable process economic benefits can be realized by incorporating these catalyst performance improvements into the process design [6]. The combination of increased productivity and decreased aromatics selectivity suggests a corresponding increase in overall carbon efficiency to desired products, which is a key driver in biomass-to-fuels process economics. Similarly, the reduction in aromatic products suggests that the catalyst may also exhibit a longer lifetime than the parent H-BEA catalyst that requires frequent regeneration [6,7]. The NREL research team continues to improve the Cu/BEA catalyst performance and optimize reaction conditions, including the C₄/isobutane recycle conversion, toward the 2022 cost goal. The catalyst performance metrics are shown in Table 3 and the results are derived from the bench-scale experiments described in the following sections.

Table 3. Summary of 2020 Experimental Performance Relative to Major Technical Targets

Process Parameter	2020 Target	2020 SOT	2022 Projection
Hydrocarbon synthesis reactor temperature	220°C–225°C	225°C	225°C
Single-pass DME conversion	39.5%	43.4%	40.0%
Productivity of hydrocarbon synthesis catalyst (kg/kg-cat/h)	0.09	0.094	0.10
Carbon selectivity to C ₅₊ product	80.1% (overall)	76.0% (single-pass)	86.7% (overall)
Carbon selectivity to aromatics	4.2% aromatics (2.2% HMB ^a)	3.2% aromatics (1.6% HMB)	0.5% aromatics (0.5% HMB)
H ₂ addition to hydrocarbon synthesis	Yes	Yes	Yes
Mixed butane (C _{4s}) handling	Recycled to hydrocarbon synthesis reactor	Recycled to hydrocarbon synthesis reactor: 58% iC ₄ recycle efficiency ^b at iC ₄ /DME ratio of 1.2	Recycled to hydrocarbon synthesis reactor: 40% recycle efficiency

^a Hexamethylbenzene

^b iC₄ recycle efficiency is defined as the reduction in iC₄ productivity with iC₄ co-fed relative to iC₄ productivity without iC₄ co-fed under otherwise identical reactor conditions.

5.1.1 Isobutane Recycle Study

Isobutane recycle and reincorporation in the hydrocarbon product to produce larger (i.e., C5+) molecules can help improve the economics of this process. NREL's SOT Cu/BEA catalyst was tested with simulated isobutane recycle experiments to quantify its effectiveness in this regard. The reaction conditions tested were 225°C, 323 kPa absolute (35 psig), a DME weight-hourly space velocity of 0.58 h⁻¹, and a DME/H₂ mol ratio of 1:1 (each at approximately 28 mol%). When iC4 was co-fed, the partial pressure of isobutane in the feed was varied between 74 and 130 kPa absolute, corresponding to ratios of approximately 1:1:0.8 to 1:1:1.4 for DME:H₂:iC₄, respectively. To aid in quantifying the effect of co-fed isobutane on catalytic performance, the catalyst was tested without co-fed isobutane (0 kPa iC₄). At this condition, argon was used as the balance gas to establish the equivalent DME and H₂ partial pressures (ca. 94 kPa absolute) as in the co-fed iC₄ conditions. The data from these experiments with and without co-fed iC₄ are presented in Table 4 and Figure 2.

Table 4. Catalyst Performance Metrics at Varying iC₄/DME Mol Ratios. For the 2020 SOT Assessment, the iC₄/DME Mol Ratio of 1.2 (Red) Was Selected for the Design Base Case.

Metric	iC ₄ /DME mol ratio				
	0	0.8	1.0	1.2	1.4
Single-pass DME Conversion (%)	51.2	35.1	44.6	43.4	48.2
Total HC productivity (kg/kg-cat/h)	0.13	0.094	0.12	0.094	0.11
C-Selectivity to C5+ (C%) (single-pass)	57.8	64.5	62.7	76.0	73.6
C-Selectivity to coke precursors (C%)	1.9	1.7	1.7	1.6	1.5
C4 Recycle Efficiency (%)	–	41	34	58	51

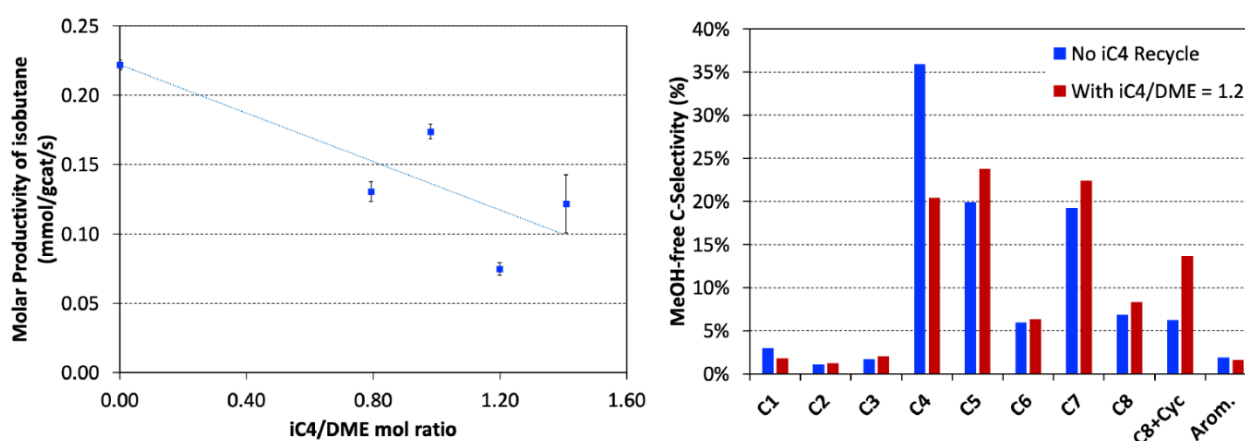


Figure 2. (Left) Molar productivity of isobutane as a function of iC₄/DME mol ratio. Error bars represent the standard error about the mean. (Right) Carbon selectivity for the 2020 SOT case at iC₄/DME mol ratios of 0 and 1.2.

5.1.2 Key Catalyst Performance Metrics and Model Assumptions

The research focus for this pathway is the conversion of DME to hydrocarbons. The key Cu/BEA catalyst performance metrics or parameters for assessing overall performance of the DME-to-

hydrocarbon conversion step are: (1) single-pass conversion of DME, (2) hydrocarbon productivity of the catalyst, (3) selectivity to desired products (C5+ hydrocarbons), (4) C4 alkane recycle efficiency, and (5) carbon selectivity to aromatics. The NREL thermochemical research team generated experimental data for the 2020 SOT performance. The 2020 experimental results for the SOT base case for the key technical performance metrics are highlighted in Table 3 and are compared against the 2020 target values and 2022 projection values. At an iC4/DME mol ratio of 1.2, the demonstrated DME single-pass conversion obtained from NREL's Cu-modified beta zeolite catalyst was 43.4% at 225°C, which exceeds the 2022 projection (40% at 225°C). Without co-fed iC4, single-pass DME conversion was demonstrated to increase at higher operating temperature, reaching 51.2% at 225°C (Table 4) [8]. Thus, there is a trade-off between single-pass DME conversion and C5+ selectivity. Experimental data in previous reports also revealed that an increased operating pressure of 20–25 psig resulted in a moderate increase in the C5+ selectivity, as well as a notable increase in the C7 product along with a corresponding decrease in C4 species (non-gasoline-range light gases) during the DME-to-hydrocarbons reaction. While the current process model includes higher-pressure (205-psia) operation and includes additional compression costs, the experimental data are limited to lower pressure due to operational constraints and leave room for future improvements by adjusting the operating conditions. Thus, the current simulated results at 205 psia can be considered conservative in the context of the improved product selectivity trend at higher pressures compared to experimental pressures of 3–35 psig.

Experiments employing a simulated C4 alkane recycle were performed, and the observed performance was compared to experiments without simulated recycle (Table 4, Figure 2). Co-fed isobutane conversion is difficult to directly measure due to concurrent isobutane production from DME. However, the overall production of isobutane was determined, and this was found to decrease when isobutane was co-fed over the range of iC4/DME mol ratios investigated here. Exploring these multiple iC4/DME co-feed ratios provides a range of data to explore in TEA scenarios to understand the effect of recycle ratio and corresponding recycle efficiency as it relates to modeled product yield and cost. With an iC4/DME mol ratio of 1.2, a 58% reduction in iC4 productivity was observed, which exceeds the 2022 projection of 40%. Under these conditions, a notable decrease in C4 selectivity was observed, with a corresponding increase in C5+ product selectivity (Figure 2, right panel). The single-pass C5+ selectivity for the 2020 SOT was found to be 76.0%, an increase over the 2018 and 2019 SOT values of 56%–72%.

Without co-fed iC4, the demonstrated hydrocarbon productivity was determined to be 0.13 kg/kg-cat/h, which exceeds the 2022 projection (0.10 kg/kg-cat/h). A small decrease was observed with co-fed iC4, with productivity values ranging from 0.094–0.12 kg/kg-cat/h. Note that catalyst productivity is affected by the interplay of multiple factors including DME conversion, C4 reactivation rate, carbon selectivity, and space velocity. The carbon selectivity to aromatics was compared between the experiments with and without co-fed C4 by assessing the ratio of C2/C5+ products, comparable to literature reports for methanol to hydrocarbons chemistry over zeolite catalysts [9–12]. A reduction in the C2/C5+ ratio was observed when isobutane was co-fed, indicating a decrease in the carbon selectivity to aromatics from 1.9% to 1.5%–1.7% under the simulated recycle conditions. From this analysis, the aromatics carbon selectivity was reduced to approximately 3.5%, with half of this attributed to HMB. HMB is removed from the catalyst surface during the catalyst regeneration under a typical oxidation condition [13]. The selectivity for the aromatics for the 2022 projection is 0.5%, representing an area of continued research.

The inclusion of experimentally simulated iC4/DME mol ratio studies eliminates extrapolation of experimental data in the process model. As such, the data set corresponding with an iC4/DME mol ratio of 1.2 was used as the design basis for the DME to HOG conversion reactor. The detailed carbon number and species selectivity distribution used in the base case assessment are summarized in Table 5.

Table 5. 2020 SOT Experimental DME to Hydrocarbons on Cu/BEA Catalyst Product Selectivity (iC4/DME = 1.2)

Carbon Number	Carbon Selectivity	Species	Species Selectivity per Carbon Number
C1	1.75%	Methane (CH ₄)	100.00%
C2	1.17%	Ethane (C ₂ H ₆)	14.47%
		Ethene (C ₂ H ₄)	85.53%
C3	1.96%	Propane (C ₃ H ₈)	33.84%
		Propene (C ₃ H ₆)	66.16%
C4	19.75%	Methylpropane (C ₄ H ₁₀)	89.12%
		n-Butane (C ₄ H ₁₀)	3.59%
		2-Methylpropene (C ₄ H ₈)	2.83%
		But-1-ene (C ₄ H ₈)	4.46%
C5	23.00%	2-Methylbutane (C ₅ H ₁₂)	97.31%
		2-Methylbutene (C ₅ H ₁₀)	2.69%
C6	6.14%	3-Methylpentane (C ₆ H ₁₄)	31.19%
		2,3-Dimethylbutane (C ₆ H ₁₄)	60.73%
		2,3-Dimethylbutene (C ₆ H ₁₂)	8.08%
C7	21.71%	2,2,3-Trimethylbutane (C ₇ H ₁₆)	45.59%
		2,4-Dimethylpentane (C ₇ H ₁₆)	26.19%
		2-Methylhexane (C ₇ H ₁₆)	22.62%
		2,2,3-Trimethylbutene (C ₇ H ₁₄)	0.30%
		2-Methyl-1-Hexene (C ₇ H ₁₄)	5.31%
C8	8.04%	2,2,4-Trimethylpentane (C ₈ H ₁₈)	89.48%
		2,4,4-Trimethyl-1-pentene (C ₈ H ₁₆)	10.52%
C8+cyc	10.22%	Dimethylcyclohexane (C ₈ H ₁₆)	24.12%
		Trimethylcyclohexane (C ₉ H ₁₈)	75.88%
C9+	2.96%	Trimethylpentane (C ₉ H ₂₀)	100.00%
Aromatics (HMB)	1.64%	Hexamethylbenzene (C ₆ (CH ₃) ₆)	100.00%
Aromatics (Others)	1.64%	Methylbenzene (C ₇ H ₈) ^a	100.00%
Total	100%		

^a Model compound representing other aromatics.

5.2 Techno-Economic Analysis Results

Table 6 summarizes key economic results for the 2020 SOT process model versus the 2022 projection. The total HOG product production rate is 37.2 million (MM) gallons of gasoline equivalent (GGE) per year (51.4 GGE/dry U.S. ton of feedstock). No liquid petroleum gas (LPG) co-product is recovered for sale in this analysis. All light end products are either recycled to the DME-to-HOG reactor for iC4 reactivation or utilized by the tar reformer combustor as fuel. The total annual operating costs and total capital investment are \$78 MM and \$407 MM, respectively, resulting in a base case MFSP for the HOG product of \$3.45/GGE.

Table 6. Summary of Process Performance and Economic Results

	2020 SOT	2022 Projection
Feedstock rate	2,205 dry U.S. ton/day	
Online time	7,884 h/yr (90% online factor)	
Total C5+ fuel yield	51.4 GGE per dry U.S. ton feedstock	54.7 GGE per dry U.S. ton feedstock
LPG coproduct	—	—
Total fuel production rate C5+ [LPG]	37.2 [0] MM GGE per year	39.6 [0] MM GGE per year
Total annual operation cost and credits	\$78 MM	\$79 MM
Total installed equipment cost	\$234 MM	\$228 MM
Total capital investment	\$407 MM	\$397 MM
Total capital investment per annual gallon	\$10.94/GGE	\$10.03/GGE
Minimum fuel selling price	\$3.45/GGE	\$3.30/GGE
Feedstock costs	\$1.23/GGE	\$1.11/GGE
Operating costs and credits	\$0.86/GGE	\$0.66/GGE
Capital charges and taxes	\$1.36/GGE	\$1.54/GGE

A cost contribution breakdown is provided in Figure 3. Feedstock costs make up about 36% (\$1.24/GGE) of the total minimum fuel selling price, with the remainder of the costs attributed to in-plant operating expenses and capital charges. The conversion of syngas to high-octane gasoline including purification steps is \$0.80/GGE, about 23% of the MFSP, with additional breakdown of these cost contributions shown in Figure 3 as the five sections from “Acid Gas Removal and Hydrogen Recovery” to “HOG Separations.” The conversion of methanol to high-octane gasoline including purification steps is \$0.45/GGE, about 13% of the MFSP (Figure 3: “MeOH Conversion to DME,” “DME Conversion to HOG,” and “HOG Separations”). Electricity is generated on-site using a combined heat and power cycle such that no electricity is imported or exported from the grid. Thus, electricity costs for each area are offset by on-site generated electricity. The process design is also self-sufficient with respect to hydrogen added to the DME-to-HOG step. A fraction of the hydrogen is extracted from the syngas before methanol synthesis (via pressure-swing adsorption) and reintroduced downstream into the DME to HOG reactor. Therefore, no additional costs or greenhouse gas penalties are incurred for hydrogen import. Finally, no LPG is recovered in the 2020 SOT analysis, and therefore coproduct credits do not contribute to the final MFSP.

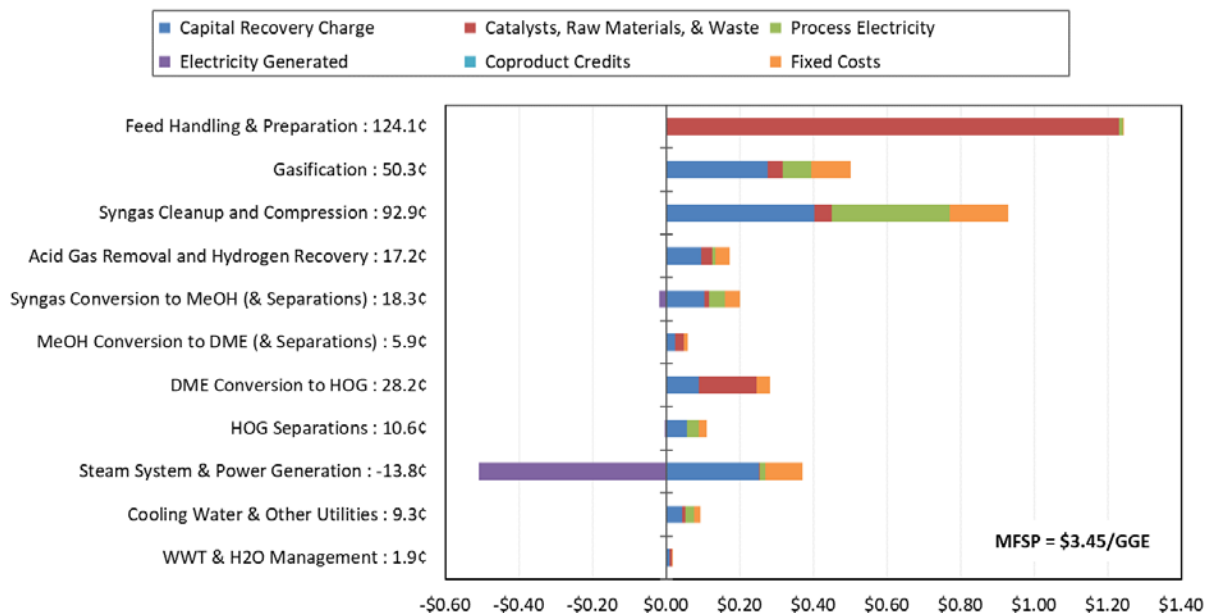


Figure 3. Cost breakdown for the 2020 SOT model

WWT = wastewater treatment

As discussed in Section 5.1.2, experimental iC4:DME ratios were studied to minimize uncertainty and eliminate the need for data extrapolation within the TEA model. The case with an iC4:DME ratio of 1.2 was selected as the base case and resulted in an MFSP of \$3.45/GGE. The metrics used to evaluate each iC4:DME condition are highlighted in Table 4. The case with an iC4:DME ratio of 0 was not evaluated in the TEA due to the comparatively low selectivity toward C5+ products and a requirement of an LPG coproduct for the iC4, both of which make this case unfavorable. The additional cases with iC4:DME ratios of 0.8, 1, and 1.4 were conducted and the summary of the results are shown in Figure 4. The iC4:DME ratio of 0.8 resulted in the highest MFSP of \$3.88/GGE. This is attributed to lower conversion and selectivity performance relative to the base case, resulting in lower yields and higher capital and operating expenses. The case with an iC4:DME ratio of 1 resulted in a slightly lower MFSP of \$3.73/GGE. In this case, C5+ selectivity was similar to the 0.8 case, but benefits were realized from increased single-pass DME conversion. The final case with an iC4:DME ratio of 1.4 had an MFSP of \$3.45/GGE, in line with the base case. In this case, slight increases to single-pass DME conversion were offset by slightly lower C5+ product selectivity.

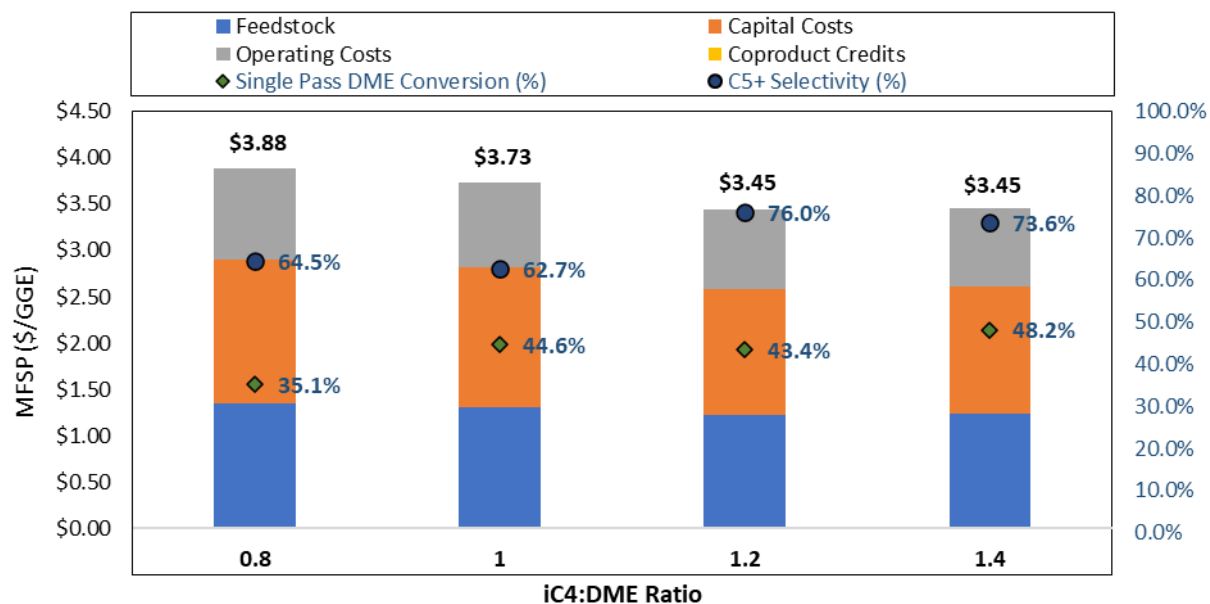


Figure 4. Results from iC4:DME ratio study

5.3 Sensitivity Analyses

Sensitivity analysis was performed on the 2020 SOT base case; effects of uncertainties related to experimental performance, capital and operating costs, and market assumptions are shown in Figure 5. The sensitivity analysis performed here is largely consistent with the sensitivity analysis completed in the 2018 SOT report [8], which was performed on the 2022 target case. Figure 5 identifies two types of variables that were tested, including market and financial parameters (shown in blue) and process parameters (shown in red). The results are shown as a percent change from the base case MFSP of \$3.45/GGE for the iC4:DME case of 1.2.

Case 1 shows the impacts of economies of scale. A larger plant feeding 10,000 dry tonnes biomass/day has the potential to achieve fuel costs 30.9% lower (\$2.38/GGE) than the currently modeled 2,000 dry tonnes biomass/day, provided the feedstock cost remains the same. Conversely, decreasing plant size to a feed rate of 600 dry tonnes biomass/day increases the MFSP to \$5.11/GGE. However, an important caveat to consider that was not included in this sensitivity case is that feedstock cost will likely trend towards lower cost at smaller scale, and higher cost a larger scale. IRR, shown in case 2, is also an important factor in determining MFSP. In a scenario assuming a 0% IRR, the MFSP is reduced to \$2.57/GGE, versus a scenario assuming an IRR of 20% yielding an MFSP of \$4.39/GGE. Other financial parameters regarding capital cost assumptions such as total capital investment and installation factor also have a noticeable impact on MFSP, as shown in case 3 and case 4. The costs of individual capital-intensive processing units were also studied as shown in cases 14, 15, 17, and 22.

Metrics relating to the performance of the DME-to-HOG conversion are of particular interest as they relate directly to the catalyst development work performed for the 2020 SOT. Case 18 indicates the impact of single-pass conversion of DME to HOG on MFSP. The results of the sensitivity case show an MFSP range of \$3.41 to \$3.51/GGE, corresponding to a 20% increase and decrease of single-pass DME conversion, respectively. This is reflective of an increase in product yield, capital cost savings

in the DME conversion to HOG step, and reduced separations cost of unconverted DME. Hydrocarbon synthesis catalyst productivity is a factor in HOG reactor scaling and capital cost estimation. Case 21 considers a $\pm 20\%$ variation in HOG catalyst productivity, resulting in an MFSP window of \$3.42–\$3.49/GGE. The cumulative results of the metrics from case 18 and case 21, along with C5+ product selectivity, were discussed previously in Figure 4. Case 11 and case 12 investigate the impacts of varying catalyst price and lifetime assumptions of the hydrocarbon synthesis catalyst.

An additional scenario was considered in which a CO₂ capture and sequestration credit is applied. In the current process design, methanol production from syngas is optimized for about 5 vol % CO₂ in the influent syngas stream. To reduce CO₂ to acceptable levels for efficient methanol synthesis, an amine acid gas removal step is employed. Captured CO₂ is assumed to be vented and treated as a zero-value waste. Because the acid gas removal equipment is already in place and produces a high-purity CO₂ stream, it is feasible that CO₂ could be sequestered via enhanced oil recovery technologies, distributed as a feedstock for technologies converting CO₂ to fuels and chemicals, or sequestered elsewhere. In the 2018 revision of the 45Q tax credit [14], the limit for facilities to be eligible for a tax credit was lowered to a minimum 100,000 tons/year of captured CO₂ (from 500,000 tons/year) [15]. The 45Q tax code specifies credit values ranging from \$50/ton and below or \$35/ton and below and depend primarily on end use of the captured CO₂ [16]. The current design captures ~300,000 tons CO₂/year, which is above the eligibility limit. As such, we applied a range of CO₂ credit values, with a maximum credit value of \$40/ton captured and a minimum value of \$0/ton captured (base case). Increments of \$10/ton were presented in the Executive Summary to account for uncertainty in compression and transportation costs, as well as uncertainty in the initial credit value. Figure 5 shows the maximum credit versus the baseline. As a result, a credit of \$40/ton yields a 9.5% reduction in MFSP, or \$3.12/GGE.

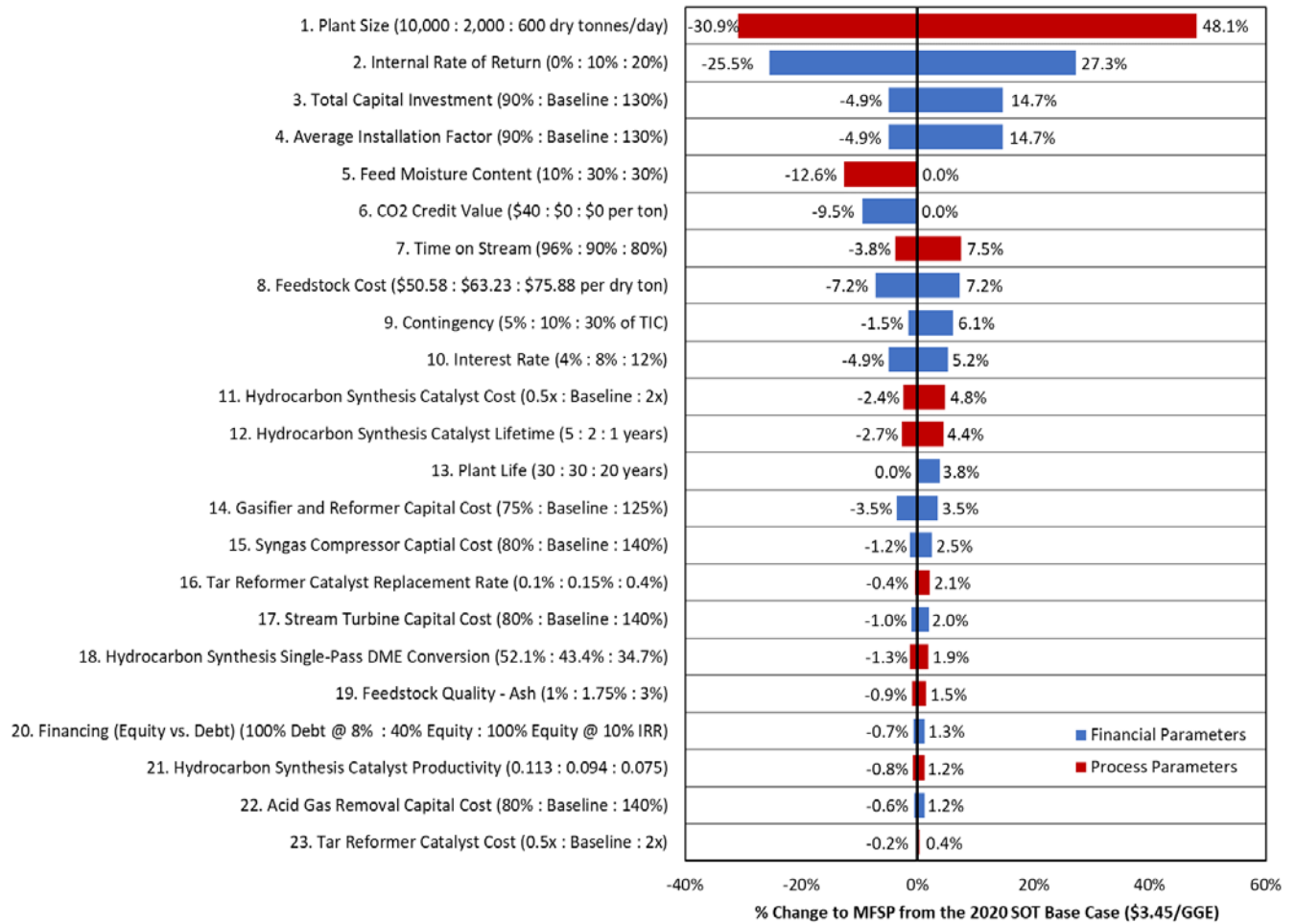


Figure 5. Sensitivity analysis for the 2020 SOT base case

6 Sustainability Assessment

The Aspen Plus models developed for the techno-economic analysis provided the material and energy results for the sustainability assessment. The sustainability metrics benchmarking the IDL-to-HOG pathway for the 2020 SOT case and the 2022 projection case were based on the products, resources, and wastes provided in Table 7. In the 2020 SOT process design, like the 2022 projection, the only fuel product is high-octane gasoline. This is different from the 2019 SOT model, in which an LPG coproduct was also obtained. In all cases, sulfur is recovered during acid-gas removal as a byproduct, and the electricity consumed and produced on-site are approximately equal, yielding a net electricity output close to 0 kWh. Table 7 also shows the direct air emissions from the biorefinery, which in addition to raw materials and products can be utilized separately by ANL for the complete supply chain sustainability analysis [17].

Table 7. Material and Energy Flows for the HOG Conversion Process (Gate-to-Gate)

Cases		2020 SOT	2022 Projection
		Production Rate	Production Rate
Products			
HOG	lb/hr	28,833	30,768
	gal/hr	5,059	5,144
	MM Btu/hr	548	583
HOG properties	LHV (Btu/gal)	108,337	113,309
	Density (g/gal)	2,585	2,713
	Biogenic C in HOG, %	100.00%	100.00%
	C content in HOG, wt%	83.90%	83.11%
Byproducts			
Mixed butanes (LPG)	lb/hr	—	—
	gal/hr	—	—
	MM Btu/hr	—	—
LPG properties	LHV (Btu/gal)	—	—
	Density (g/gal)	—	—
	Biogenic C in HOG, %	—	—
	C Content in HOG, wt%	—	—
Sulfur	lb/hr	116	114
Excess electricity	kWh	5	(36)
Resource Consumption		Flow Rate (lb/hr)	Flow Rate (lb/hr)
Blended woody biomass (wet)		262,455	262,455
Blended woody biomass (dry)		183,718	183,718
Magnesium oxide (MgO)		13.3	23
Fresh olivine		539	527
Tar reformer catalyst		9.5	9
Natural gas for reformer		0.0	0
Methanol synthesis catalyst		4.6	5
DME catalyst		8.8	6

Cases	2020 SOT	2022 Projection
Beta zeolite catalyst	39.0	34
Zinc oxide catalyst	2.5	2.5
Shift catalyst	0.2	0
Cooling tower water makeup	54,291	31,213
Boiler feedwater makeup	10,233	86,887
Other freshwater makeup ^a	64,206	0
Dimethyl disulfide (DMDS)	2.1	2.1
Amine (MDEA) makeup	4.2	3.7
LO-CAT chemicals	116	114
Boiler feedwater chemicals	2.7	2.7
Cooling tower chemicals	1.5	1.0
No. 2 diesel fuel	69.2	69
Waste Streams	lb/hr	lb/hr
Sand and ash purge	4,129	6,679
Tar reformer catalyst	8.7	8.7
Scrubber solids	116	8.8
Wastewater	2,537	14,845
Air Emissions	lb/hr	lb/hr
CO ₂ (biogenic)	246,881	241,844
CO ₂ (fossil)	0	0
CH ₄	0	0
CO	0	0
NO ₂	77	142
SO ₂	52	51
H ₂ O	138,168	73,422
H ₂ S	1	0
Heating Values of Fuel to Combustors	MM Btu/hr	MM Btu/hr
<i>Char combustor</i>		
LHV to char combustor	436	528
HHV to char combustor	453	553
Char combustor % biogenic C	100%	100%
<i>Fuel combustor</i>		
LHV to fuel combustor	395	235
HHV to fuel combustor	432	254
Fuel combustor % biogenic C	100%	100%

^a Other freshwater makeup includes methanol wash water and makeup for the flue gas scrubber in 2020 case

The inputs and outputs provided in Table 7 were used to derive the sustainability metrics summarized in Table 8. The results are shown for the 2019 SOT, 2020 SOT, and the 2022 projection cases. As previously discussed, the 2020 SOT case does not include an LPG coproduct. As a result,

the overall gallons of gasoline equivalent produced in the 2020 SOT is higher than the 2019 SOT case, because the 2020 case has a greater carbon efficiency to HOG (24.8% in the 2019 SOT case versus 26% in the 2020 SOT case). The 2020 SOT HOG yield is 51.4 GGE/dry U.S. ton biomass, compared to the 2022 projection of 54.7 GGE/dry U.S. ton biomass. A portion of the syngas produced from biomass is combusted to supplement the steam-turbine combined heat and power system such that the net electricity import is negligible and no natural gas is required. Direct water consumption of the process includes evaporative losses from the cooling tower and flue gas scrubber, steam system blowdown, and methanol wash wastewater. The 2020 SOT case shows an increase in water consumption to 3.3 gal/GGE compared to the 2019 SOT of 2.9 gal/GGE. The overall greenhouse gas reduction of the IDL-derived fuels relative to petroleum-derived fuels is 78% for the 2020 SOT case, equal to that of the 2019 SOT case. The complete sustainability analysis results for both the 2019 SOT and 2020 SOT were conducted by ANL and are reported separately [17, 18].

Table 8. Summary of Sustainability Metric Indicators for the 2019 SOT, 2020 SOT, and 2022 Projection Cases

Sustainability Metrics	Units	2019 SOT	2020 SOT	2022 Projection
HOG fuel yield by weight of biomass	GGE per dry U.S. ton biomass	49	51.4	54.7
LPG fuel yield by weight of biomass	GGE per dry U.S. ton biomass	5.6	—	—
Carbon efficiency to HOG + LPG	% C in feedstock	24.8 + 2.3	26 + 0	28 + 0
Electricity import	kWh/GGE	— ^a	— ^a	— ^a
Natural gas import	MJ/GGE	— ^b	— ^b	— ^b
Water consumption	gal/GGE	2.9	3.3	2.8
Water consumption	m ³ /day	1,258	1,406	1,286

^a Negligible

^b No natural gas import

7 Conclusions and Future Work

This report is an update on the research and development progress for the indirect liquefaction of biomass to high-octane gasoline through a methanol and dimethyl ether intermediates. Together, the 2020 SOT experimental and TEA results are used to measure the pathway's progress toward the 2022 performance and cost targets and provide recommendations for future work. Specific emphasis was placed on improvements to the performance of NREL's Cu/BEA catalyst. Unique to this year's assessment, iC4 reactivation was studied via the use of simulated recycle experiments under various iC4/DME mol ratios. These key studies reduced model uncertainties via the elimination of data extrapolation for DME to HOG with iC4 recycle and reactivation. An overall decrease in aromatics production and reincorporation of C4 products into C5+ (HOG) products led to an increase in overall HOG yield over the 2019 SOT figure (Table ES-1). Catalyst performance improvements under these process conditions, in conjunction with significant process model optimization, led to a final MFSP of \$3.45/GGE, surpassing 2020 SOT projections (\$3.49/GGE). This work also highlighted the impact of incentives and potential for cost reduction through CO₂ capture credits.

Future work will continue to pursue improved catalyst performance metrics, specifically in the realm of DME conversion to HOG. Key metrics include reduced aromatics formation, with a 2022 target value of 0.5% aromatics selectivity, and increased DME conversion to C5+ products. Increasing DME single-pass conversion and catalyst productivity to HOG will put 2022 MFSP cost targets (\$3.30/GGE) within reach. Additional efforts will look to identify methods for improving environmental performance metrics such as carbon efficiency. Potential routes for improvement in this area could include CO₂ reincorporation into products or overall process optimization to reduce energy consumption. Future experimentation of DME conversion at elevated pressures to match the process model assumptions will likely boost DME-to-HOG yields and help improve the economics.

8 References

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Appendix: Supplemental Information for SOT and Projection Cases

Table A-1. Detailed Cost Breakdown of SOT/Projection for Syngas Conversion High-Octane Gasoline Pathway

Processing Area Cost Contributions & Key Technical Parameters	Units	2014 SOT †	2015 SOT †	2016 SOT †	2017 SOT †	2018 SOT †	2019 SOT †	2020 SOT †	2021 Projection	2022 Projection (Design Case)
Process Concept: Gasification, Syngas Cleanup, Methanol / DME Synthesis & Conversion to HCs										
C ₂₊ Minimum Fuel Selling Price (per Actual Product Volume) ▲	\$ / Gallon	Woody Feedstock \$4.31	Woody Feedstock \$4.17	Woody Feedstock \$3.85	Woody Feedstock \$3.67	Woody Feedstock \$3.66	Woody Feedstock \$3.35	Woody Feedstock \$3.22	Woody Feedstock \$3.30	Woody Feedstock \$3.22
Mixed C ₂₊ 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	\$3.40	\$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	\$2.25	\$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	\$10.03	\$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 ₂₊) Yield	Gallons / Dry Ton	36.2	36.4	51.4	50.0	51.4	51.6	55.1	55.1	56.0
Mixed C ₂₊ 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	\$1.14	\$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	\$1.14	\$1.12
Feedstock Cost	\$ / Dry US Ton	\$60.58	\$60.58	\$60.58	\$57.28	\$60.54	\$63.23	\$63.23	\$60.54	\$60.54
Ash Content	wt % Ash	3.00%	3.00%	3.00%	3.00%	3.00%	1.75%	1.75%	3.00%	3.00%
Feedstock Moisture at Plant Gate	Wt % H ₂ O	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	\$0.69	\$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 ₂ O	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	7,856	7,856
Gasification										
Total Cost Contribution	\$ / Gallon GE	\$0.69	\$0.67	\$0.65	\$0.62	\$0.61	\$0.58	\$0.50	\$0.56	\$0.54
Capital Cost Contribution	\$ / Gallon GE	\$0.43	\$0.41	\$0.38	\$0.35	\$0.34	\$0.33	\$0.28	\$0.31	\$0.30
Operating Cost Contribution	\$ / Gallon GE	\$0.26	\$0.26	\$0.27	\$0.28	\$0.26	\$0.25	\$0.23	\$0.25	\$0.24
Raw Dry Syngas Yield	lb / lb Dry Feed	0.76	0.76	0.76	0.76	0.76	0.77	0.83	0.76	0.76
Raw Syngas Methane (Dry Basis)	Mole %	15.4%	15.4%	15.4%	15.4%	15.4%	15.4%	8.6%	15.4%	15.4%
Gasifier Efficiency (LHV)	% LHV	71.9%	71.9%	71.9%	71.9%	71.9%	72.3%	78.0%	71.9%	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	\$0.80	\$0.78
Capital Cost Contribution	\$ / Gallon GE	\$0.51	\$0.49	\$0.46	\$0.43	\$0.41	\$0.39	\$0.40	\$0.37	\$0.36
Operating Cost Contribution	\$ / Gallon GE	\$0.45	\$0.45	\$0.48	\$0.51	\$0.48	\$0.49	\$0.53	\$0.44	\$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%	1.7%	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%

Processing Area Cost Contributions & Key Technical Parameters	Units	2014 SOT †	2015 SOT †	2016 SOT †	2017 SOT †	2018 SOT †	2019 SOT †	2020 SOT †	2021 Projection	2022 Projection (Design Case)
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	\$0.41	\$0.40
Capital Cost Contribution	\$ / Gallon GE	\$0.35	\$0.33	\$0.30	\$0.28	\$0.28	\$0.27	\$0.20	\$0.25	\$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	0.7	0.7
Methanol Intermediate Yield	Gallons / Dry Ton	143	142	138	144	141	137	150	136	134
Hydrocarbon Synthesis										
Total Cost Contribution	\$ / Gallon GE	\$0.91	\$0.91	\$0.70	\$0.67	\$0.64	\$0.49	\$0.34	\$0.51	\$0.48
Capital Cost Contribution	\$ / Gallon GE	\$0.56	\$0.56	\$0.46	\$0.44	\$0.42	\$0.34	\$0.11	\$0.34	\$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	145	145
Hydrocarbon Synthesis Reactor Pressure	psia	129	129	129	129	129	129	205	129	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 relative to aromatics						
Utilization of C ₄ in Reactor Outlet via Recycle		0%	0%	100%	100%	100%	90%	97%	Recycle	100%
Single-Pass DME Conversion	%	15.0%	15.0%	19.2%	27.6%	38.9%	44.7%	43.4%	39.7%	40.0%
Overall DME Conversion	%	83%	85%	83%	88%	92%	88%	96%	90%	90%
Hydrocarbon Synthesis Catalyst Productivity	kg / kg-cat / hr	0.02	0.03	0.04	0.09	0.07	0.07	0.07	0.09	0.10
Carbon Selectivity to C ₂₊ Product	% C in Reactor Feed	46.2%	48.3%	81.8%	74.8%	72.3%	73.6%	72.1%	83.4%	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%	2.4%	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%	1.4%	0.5%
Hydrocarbon Product Separation										
Total Cost Contribution	\$ / Gallon GE	\$0.04	\$0.05	\$0.05	\$0.05	\$0.05	\$0.05	\$0.11	\$0.05	\$0.05
Capital Cost Contribution	\$ / Gallon GE	\$0.03	\$0.03	\$0.04	\$0.04	\$0.04	\$0.03	\$0.06	\$0.03	\$0.03
Operating Cost Contribution	\$ / Gallon GE	\$0.01	\$0.01	\$0.01	\$0.01	\$0.01	\$0.01	\$0.05	\$0.01	\$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)	(\$0.08)	(\$0.07)
Capital Cost Contribution	\$ / Gallon GE	\$0.42	\$0.40	\$0.36	\$0.34	\$0.33	\$0.29	\$0.31	\$0.29	\$0.28
Operating Cost Contribution	\$ / Gallon GE	(\$0.41)	(\$0.42)	(\$0.42)	(\$0.45)	(\$0.42)	(\$0.41)	(\$0.33)	(\$0.37)	(\$0.36)
Sustainability and Process Efficiency Metrics										
Carbon Efficiency to C ₂₊ Product	% C in Feedstock	19.3%	19.4%	25.2%	24.3%	25.5%	24.8%	26.1%	27.4%	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%	27.4%	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%	39.6%	40.4%
Electricity Production	kWh / Gallon C ₂₊	11.7	11.8	7.9	8.4	8.1	7.6	12.2	7.2	7.0
Electricity Consumption	kWh / Gallon C ₂₊	11.7	11.8	7.9	8.5	8.1	7.6	12.2	7.2	7.0
Water Consumption	Gal H ₂ O / Gal C ₂₊	12.9	10.1	3.1	3.3	3.2	2.9	3.3	2.8	2.8
TEA Reference File		2014 SOT Rev4a 2016s (high ash)_1.xlsx	2015 SOT Rev6 Comm-HBEA 2016s FR Rev2_1.xlsx	2016 SOT Base Rev6 Rev2 2016s FR_1.xlsx	2017 SOT Base Rev1 2016s FR_1 KH (Feedstock Cost).xlsx	2018SOT_2018-07-20data Rev3_2 KH (Feedstock Cost).xlsx	2019 SOT Oct Update Rev02 - (C4-DME-1_LPG) Rev0_b.xlsx	HOG2020-V117_rev5.xlsx	2021 Target Rev0 KH (Feedstock Cost).xlsx	2022 Design FR Rev5a_2 KH (Feedstock Cost).xlsx

▲ Conceptual design result

† SOT: state of technology.

Minimum Fuel Selling Price (MFSP) Breakdown (\$ / Gallon of Gasoline Equivalent)	2014 State of Technology	2015 State of Technology	2016 State of Technology	2017 State of Technology	2018 State of Technology	2019 State of Technology	2020 State of Technology	2021 Projection	2022 Projection (Design Case)
Gasification	\$ 0.69	\$ 0.67	\$ 0.65	\$ 0.62	\$ 0.61	\$ 0.58	\$ 0.50	\$ 0.56	\$ 0.54
Synthesis Gas Clean-up (Reforming and Quench)	\$ 0.96	\$ 0.93	\$ 0.94	\$ 0.94	\$ 0.89	\$ 0.88	\$ 0.93	\$ 0.80	\$ 0.78
Acid Gas Removal, Methanol Synthesis and Methanol Conditioning	\$ 0.52	\$ 0.50	\$ 0.47	\$ 0.47	\$ 0.45	\$ 0.45	\$ 0.36	\$ 0.41	\$ 0.40
Hydrocarbon Synthesis	\$ 0.91	\$ 0.91	\$ 0.70	\$ 0.67	\$ 0.64	\$ 0.49	\$ 0.34	\$ 0.51	\$ 0.48
Hydrocarbon Product Separation	\$ 0.04	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.11	\$ 0.05	\$ 0.05
LPG Coproduct Credit	\$ -	\$ -	\$ -	\$ -	\$ -	\$ (0.11)	\$ (0.00)	\$ -	\$ -
Balance of Plant	\$ 0.01	\$ (0.02)	\$ (0.05)	\$ (0.11)	\$ (0.09)	\$ (0.11)	\$ (0.03)	\$ (0.08)	\$ (0.07)
Minimum Fuel Selling Price (MFSP)	\$ 3.13	\$ 3.03	\$ 2.76	\$ 2.64	\$ 2.56	\$ 2.23	\$ 2.21	\$ 2.25	\$ 2.18

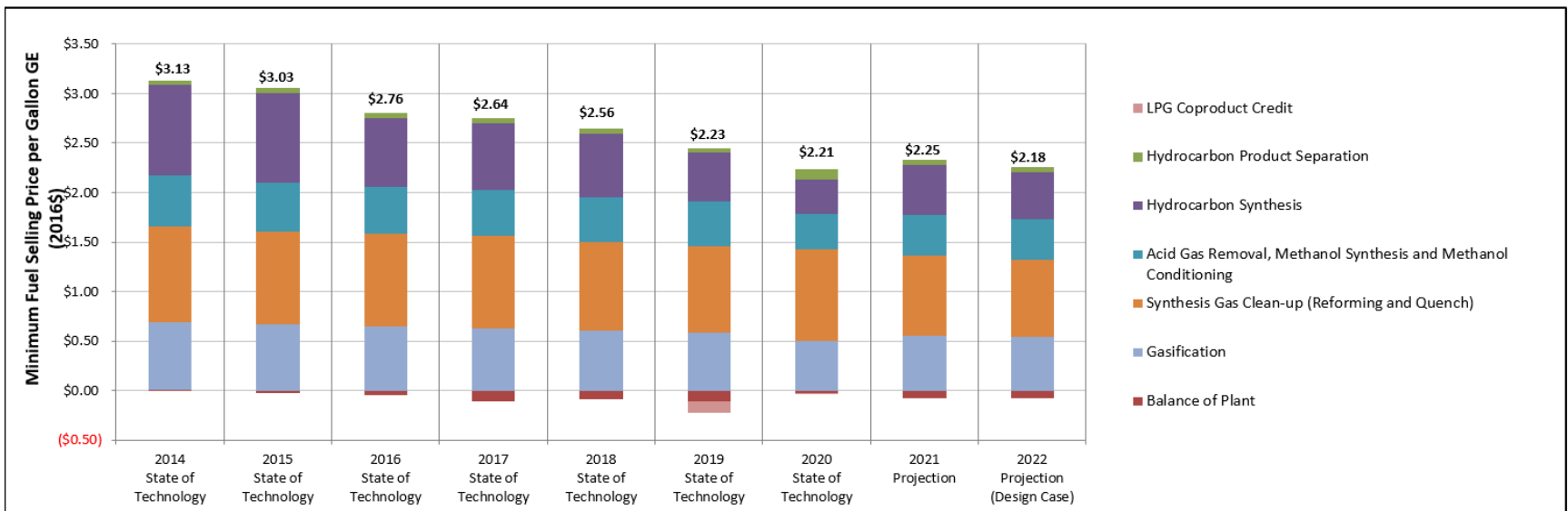


Figure A-1. SOT/waterfall for syngas conversion high-octane gasoline pathway (excluding feedstock costs) in 2016\$

Minimum Fuel Selling Price (MFSP) Breakdown (\$ / Gallon of Gasoline Equivalent)	2014 State of Technology	2015 State of Technology	2016 State of Technology	2017 State of Technology	2018 State of Technology	2019 State of Technology	2020 State of Technology	2021 Projection	2022 Projection (Design Case)
Feedstock	\$ 1.20	\$ 1.21	\$ 1.24	\$ 1.22	\$ 1.23	\$ 1.31	\$ 1.24	\$ 1.14	\$ 1.12
Gasification	\$ 0.69	\$ 0.67	\$ 0.65	\$ 0.62	\$ 0.61	\$ 0.58	\$ 0.50	\$ 0.56	\$ 0.54
Synthesis Gas Clean-up (Reforming and Quench)	\$ 0.96	\$ 0.93	\$ 0.94	\$ 0.94	\$ 0.89	\$ 0.88	\$ 0.93	\$ 0.80	\$ 0.78
Acid Gas Removal, Methanol Synthesis and Methanol Conditioning	\$ 0.52	\$ 0.50	\$ 0.47	\$ 0.47	\$ 0.45	\$ 0.45	\$ 0.36	\$ 0.41	\$ 0.40
Hydrocarbon Synthesis	\$ 0.91	\$ 0.91	\$ 0.70	\$ 0.67	\$ 0.64	\$ 0.49	\$ 0.34	\$ 0.51	\$ 0.48
Hydrocarbon Product Separation	\$ 0.04	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.05	\$ 0.11	\$ 0.05	\$ 0.05
LPG Coproduct Credit	\$ -	\$ -	\$ -	\$ -	\$ -	\$ (0.11)	\$ (0.00)	\$ -	\$ -
Balance of Plant	\$ 0.01	\$ (0.02)	\$ (0.05)	\$ (0.11)	\$ (0.09)	\$ (0.11)	\$ (0.03)	\$ (0.08)	\$ (0.07)
Minimum Fuel Selling Price (MFSP)	\$ 4.33	\$ 4.24	\$ 3.99	\$ 3.86	\$ 3.79	\$ 3.53	\$ 3.45	\$ 3.40	\$ 3.30

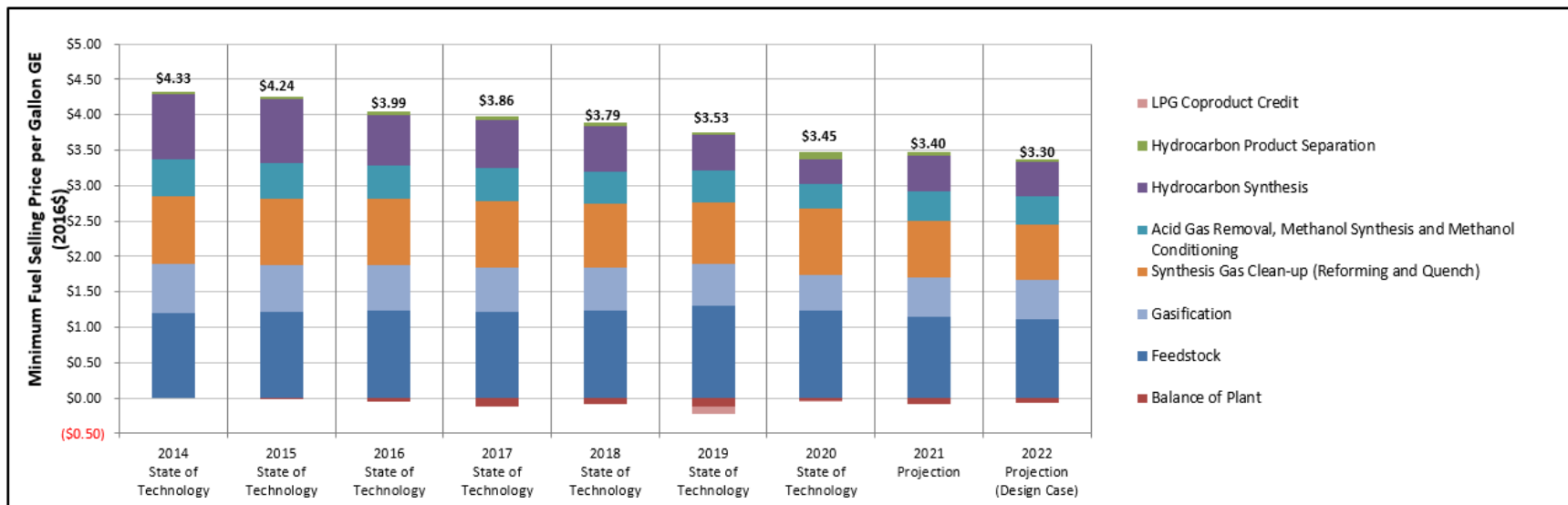


Figure A-2. SOT/waterfall for syngas conversion high-octane gasoline pathway in 2016\$