High-Octane Gasoline From Lignocellulosic Biomass via Syngas and Methanol/Dimethyl Ether Intermediates: 2021 State of Technology

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1 National Renewable Energy Laboratory
2 Idaho National Laboratory
3 Argonne National Laboratory

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Suggested Citation

NOTICE

Acknowledgments

Nomenclature

ANL	Argonne National Laboratory
BETO	Bioenergy Technologies Office
Btu	British thermal unit
DME	dimethyl ether
FY	fiscal year
GC	gas chromatography
GGE	gallon of gasoline equivalent
GHG	greenhouse gas
HHV	higher heating value
HMB	hexamethylbenzene
HOG	high-octane gasoline
iC4	isobutane
IDL	indirect liquefaction
IRR	internal rate of return
LHV	lower heating value
LPG	liquid petroleum gas
MeOH	methanol
MFSP	minimum fuel selling price
NREL	National Renewable Energy Laboratory
SAF	sustainable aviation fuel
SOT	state of technology
STH	syngas to hydrocarbons
TEA	techno-economic analysis
VUV	vacuum ultraviolet spectroscopy

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. It details the 2021 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 results of the fiscal year 2021 (FY21) SOT assessment address the technical progress of the IDL pathway toward achieving the 2022 cost target of $3.30 per gallon of gasoline equivalent (GGE), while also attaining 80% greenhouse gas (GHG) emissions reduction relative to the fossil baseline. In this year's assessment, experimental efforts utilizing the largest bench-scale reactor system to date (approximately 430-cm^3 catalyst bed) equipped with a continuous distillation unit targeted a rigorous measurement of aromatics selectivity during hydrocarbon synthesis. Detailed analytical work was conducted on the liquid hydrocarbon product to quantify aromatic selectivity. The analysis found that the carbon selectivity of dimethyl ether (DME) to total aromatics was 1.6%, a significant reduction from the estimated 3.3% in FY20. The mass balance was calculated based on reactants fed and products formed (liquid and gaseous) and closed to within 6.5% (compared to >10% using only gas-phase gas chromatography analysis). In addition to aromatics production, further research efforts were carried out to explore regeneration conditions required for reactivation of the Cu/BEA catalyst. These studies determined that the Cu/BEA catalyst can be regenerated at lower temperatures than other zeolites, suggesting that the Cu/BEA catalyst lifetime resembles that of robust Cu catalysts rather than more sensitive zeolites. Thus, the lifetime of the catalyst is extended in the model. For the purposes of the FY21 assessment, the Cu/BEA zeolite lifetime was increased from 2 years, as used in previous assessments, to 3 years. This assumption reduced the minimum fuel selling price (MFSP) by $0.05/GGE in this year's assessment, helping to achieve a lower MFSP. Finally, communications with an engineering firm identified the opportunity to reduce the excess air requirement in process combustors from 20% to 10% excess over stoichiometric requirement for complete combustion. This modification was implemented in the Aspen Plus model for the char combustor, tar reformer combustor, and catalyst regenerator.

The FY21 SOT employed the same base case performance metrics as those outlined in the FY20 SOT, including single-pass DME conversion and overall product selectivity. Hydrocarbon selectivity was updated to accommodate the lower aromatics formation. The reduced aromatics value, improved Cu/BEA catalyst lifetime, and reduced excess air requirement were all employed to determine the FY21 SOT base case. A summary of the key performance metrics from the FY20 SOT, FY21 SOT, and FY22 projection is shown in Table ES-1. Single-pass DME conversion remained at 43.4%, surpassing the FY22 projection, while the reduction in aromatics selectivity resulted in a corresponding increase in C_5+ product selectivity to 73.3%. Product selectivity data was based on current understanding of the product distribution and requires verification through further efforts towards completing mass and carbon balance closures. The overall effect of the aforementioned modifications resulted in a MFSP for the FY21 SOT of $3.38/GGE, thus meeting the $3.40/GGE target. Supply chain sustainability metrics were determined by Argonne National Laboratory (ANL), and the calculated GHG emission intensity

of the FY21 SOT case was 18 g CO_2e/MJ. This corresponds to an 80% reduction in GHG emissions relative to the fossil baseline, surpassing the 60% reduction target. More detailed descriptions of the metrics listed in Table ES-1 and their implications are provided within the main text of the report. Additionally, detailed cost breakdown summaries are provided for both the FY21 SOT case and the FY22 projection case in Table ES-1 and Table ES-2, respectively. A summary of key technical metrics achieved in the current and previous SOT, and those projected for the 2022 target case, are presented in the Appendix.

A series of single-point sensitivity cases were conducted on the FY21 SOT base case to project a range in the MFSP that accounts for process uncertainties and variations. To address uncertainty associated with imperfect mass balance closure, high- and low-C_5+ hydrocarbon cases were conducted and resulted in MFSPs of \$3.32/GGE and \$3.55/GGE, respectively. A ±20% variation of the hydrocarbon synthesis catalyst productivity resulted in an MFSP range of \$3.36–\$3.41/GGE. Another case varied aromatic selectivity from the base case value of 1.6% to 1% and 3% and resulted in MFSPs of \$3.36/GGE and \$3.40/GGE, respectively. Growing prevalence of carbon capture sequestration and utilization incentives motivated a sensitivity case to address the potential value of a 45Q carbon capture tax credit. Practiced for nearly a century, amine scrubbing technologies are highly mature and applicable for carbon capture efforts. Coupled with similarly mature carbon sequestration technologies these processes can play an important role in decarbonization in the near-term (Mac Dowell et al. 2017). Per the 45Q description, this facility would be eligible to receive up to a \$50/ton CO_2 credit if the CO_2 removed during the acid gas removal step was captured rather than released to the atmosphere. To account for additional purification and compression costs, a maximum \$40/ton CO_2 captured credit value was applied in this assessment and resulted in an MFSP of \$3.05/GGE, a \$0.33/GGE decrease from the baseline value. Thus, application of a CO_2 credit could mitigate the impacts of high-cost scenarios such as low-C_5+ hydrocarbon yield or low hydrocarbon synthesis catalysis productivity.

Table ES-1. Performance Metrics for the 2020 SOT, 2021 SOT, and 2022 Projection

Performance Metrics	2020 SOT	2021 SOT	2022 Projection
DME Conversion (%)[a]	43.4	43.4	40
C_5+ C-Selectivity (%)[b]	72.07	73.34	86.7
Aromatics C-Selectivity (%)	3.3	1.6	0.5
HOG Hydrocarbon Productivity (kg/kg-catalyst/h)	0.09	0.09	0.1
HOG Product Yield (GGE/dry U.S. ton)	51.4	51.7	54.7
Liquid Petroleum Gas Coproduct (GGE/dry U.S. ton)	—	—	—
MFSP (\$/GGE; 2016\$)	3.45	3.38	3.30
Fuel Synthesis and Separation Cost (¢/GGE; 2016\$)[c]	45	40	48
Supply Chain GHG Emissions (g CO_2e/MJ)[d]	19	18	14

[a] Single-pass conversion

[b] Overall selectivity

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As the IDL SOT cases approach the FY22 target MFSP and maintain favorable GHG emission results, future work will aim to fine-tune catalyst development and identify pathways for scale-up and commercial development with industry partners. Further, key learnings from the DME-to-HOG catalyst research will be leveraged in future efforts to develop and assess high impact process modifications including the exploration of a single-step syngas-to-hydrocarbons technology. The envisioned process contains only one reactor converting syngas directly to hydrocarbons versus the current three-step conversion process. Preliminary data for the single-step pathway indicated high CO conversion and high C4+ product selectivity. This product slate is also highly conducive for sustainable aviation fuel (SAF) production. Future research into the single-step pathway will aim to maintain high conversion and selectivity, and to activate and convert co-fed CO_2 to improve carbon efficiency to hydrocarbon products. Additionally, the process intensification of the single-step technology has the potential for reduced capital investment through fewer unit operations and higher-pressure operation.

Table ES-1. Economic Summary for 2021 SOT

Process Engineering Analysis for High Octane Gasoline via Indirect Gasification and Methanol Intermediate : 2021 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 (MFSP, Gasoline-Equivalent Basis)		$3.38 per GGE
Feedstock & In-Plant Handling Costs		1.223 per GGE
Operating Costs & Credits		0.804 per GGE
Capital Charges & Taxes		1.350 per GGE
Fuel Production at Operating Capacity		37.45 MM GGE per Year
Fuel Product Yield		51.72 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

Area A100: Feed Handling & Preparation	$200,000
Area A200: Gasification	$47,200,000
Area A300: Syngas Cleanup and Compression	$69,200,000
Area A400: Acid Gas Removal and Hydrogen Recovery	$16,800,000
Area A400SM: Syngas Conversion to MeOH (& Separations)	$18,200,000
Area A400MD: MeOH Conversion to DME (& Separations)	$4,300,000
Area A400DH: DME Conversion to HOG	$15,500,000
Area A400HCND: HOG Separations	$9,900,000
Area A600: Steam System & Power Generation	$43,100,000
Area A700: Cooling Water & Other Utilities	$7,500,000
Area A800: WWT & H2O Management	$1,800,000
Total Installed Equipment Cost (TIC)	**$233,700,000**
ISBL (Areas A100 to A400)	$171,400,000
OSBL (Areas A600 to A700)	$60,500,000
Other Direct Costs	$7,300,000
(% of ISBL)	4.0%
Total Direct Costs (TDC)	$241,000,000
Indirect Costs	$144,600,000
(% of TDC)	60.0%
Land Purchase Cost	1,600,000
Working Capital	19,300,000
Total Capital Investment (TCI)	406,500,000
Installed Equipment Cost per Annual Gallon	$6.24
Total Capital Investment per Annual Gallon	$10.85
Debt Financing (% of Investment)	60.0%
Loan Interest Rate	8.0%
Loan Term (years)	10.0
Equity Financing (% of Investment)	40.0%
Internal Rate of Return (After-Tax)	10.0%
Plant Operating Hours per year	7,884
On-Stream Percentage	90.0%

Process Efficiency

Gasifier Efficiency - HHV %	79.0
Gasifier Efficiency - LHV %	78.5
Efficiency to Gasoline - HHV %	38.2
Efficiency to Gasoline - LHV %	37.9
Overall Plant Efficiency - HHV %	38.2
Overall Plant Efficiency - LHV %	37.9

Excel File: HOG2021-V006b-air excess red_3yr.xlsm

Annual Operating Costs

Feedstock	$45,800,000
Natural Gas	$0
Catalysts	$7,200,000
Olivine	$600,000
Other Raw Matl. Costs	$1,500,000
Waste Disposal	$1,000,000
Electricity Transfer Charge	$0
Electricity	$0
Fixed Costs	$19,900,000
Coproduct credits (including electricity)	$0
Capital Depreciation	$12,900,000
Average Income Tax	$3,600,000
Average Return on Investment	$34,100,000

Operating Costs per Product	(¢/MMBtu)	(¢/GGE)
Feedstock	1053.2	122.3
Natural Gas	0.0	0.0
Catalysts	165.3	19.2
Olivine	13.1	1.5
Other Raw Materials	35.0	4.1
Waste Disposal	22.8	2.6
Electricity Transfer	0.0	0.0
Electricity	0.0	0.0
Fixed Costs	456.8	53.0
Coproduct credits	-0.4	0.0
Capital Depreciation	296.7	34.4
Average Income Tax	82.5	9.6
Average Return on Investment	783.9	91.0
Total (Plant Gate Price)	**2908.8**	**337.69**

Power Balance	(KW)	(hp)
Total Plant Power Consumption (KW)	42,101	56,458
Power Generated Onsite (KW)	42,098	56,454
Power Imported from Grid (KW)	3	4
Power Exported to Grid (KW)	0	0

Power Generation	(KW)	(hp)
Steam Turbine Generators	40,299	54,041
Process Gas Turboexpander(s)	1,799	2,413

Sustainability Metrics

Plant Electricity Consumption (KWh/ GGE)	8.9
Gasification & Reforming Steam (lb / GGE)	23.3
Water Consumption (Gal Water / GGE)	3.26
Carbon Conversion Efficiency (C in Fuel/C in Feedstock)	26.18%

Feedstock Rate and Cost

Feed Rate	Dry Tonnes / Day	2,000
	Dry US Tons / Day	2,205
Feedstock Cost	$ / Dry Ton	$63.23
	$ / Moisture & Ash Free Ton	$64.36

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Table ES-2. 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

Capital Costs

Feed Handling & Drying	$200,000
Gasification	$44,600,000
Gas Cleanup	$52,800,000
Methanol Synthesis	$33,700,000
Methanol Conditioning	$2,300,000
DME & Hydrocarbons Conversion	$47,300,000
Gasoline Separations	$5,000,000
Steam System & Power Generation	$34,700,000
Cooling Water & Other Utilities	$7,200,000
Total Installed Equipment Cost (TIC)	$227,800,000
ISBL (Areas A100 to A500, A1400, A1500)	$185,900,000
OSBL (Areas A600, A700)	$41,900,000
Other Direct Costs	7,400,000
(% of ISBL)	4.0%
Total Direct Costs (TDC)	235,265,659
Indirect Costs	141,200,000
(% of TDC)	60.0%
Land Purchase Cost	1,600,000
Working Capital	18,800,000
Total Capital Investment (TCI)	396,900,000
Installed Equipment Cost per Annual Gallon	$5.62
Total Capital Investment per Annual Gallon	$9.79
Debt Financing (% of Investment)	60.0%
Loan Interest Rate	8.0%
Loan Term (years)	10.0
Equity Financing (% of Investment)	40.0%
Internal Rate of Return (After-Tax)	10.0%
Plant Operating Hours per year	7,884
On-Stream Percentage	90.0%

Process Efficiency

Gasifier Efficiency - HHV %	72.3
Gasifier Efficiency - LHV %	71.9
Efficiency to Gasoline - HHV %	40.7
Efficiency to Gasoline - LHV %	40.4
Overall Plant Efficiency - HHV %	40.7
Overall Plant Efficiency - LHV %	40.4

Annual Operating Costs

Feedstock	$43,800,000
Natural Gas	$0
Catalysts	$11,700,000
Olivine	$600,000
Other Raw Matl. Costs	$1,500,000
Waste Disposal	$1,600,000
Electricity Transfer Charge	$0
Electricity	$0
Fixed Costs	$19,500,000
Coproduct credits	$0
Capital Depreciation	$12,500,000
Average Income Tax	$3,900,000
Average Return on Investment	$44,500,000

Operating Costs per Product

	(¢/MMBtu)	(¢/GGE)
Feedstock	954.0	110.8
Natural Gas	0.0	0.0
Catalysts	59.6	6.9
Olivine	12.1	1.4
Other Raw Materials	33.1	3.8
Waste Disposal	34.7	4.0
Electricity Transfer	0.0	0.0
Electricity	0.0	0.0
Fixed Costs	424.8	49.3
Coproduct credits	0.0	0.0
Capital Depreciation	272.0	31.6
Average Income Tax	84.4	9.8
Average Return on Investment	968.6	112.4
Total (Plant Gate Price)	2843.3	330.1

Power Balance

	(KW)	(hp)
Total Plant Power Consumption (KW)	36,084	48,389
Power Generated Onsite (KW)	36,049	48,342
Power Imported from Grid (KW)	35	47
Power Exported to Grid (KW)	0	0

Power Generation

	(KW)	(hp)
Steam Turbine Generators	34,419	46,157
Process Gas Turboexpander(s)	1,630	2,186

Sustainability Metrics

Plant Electricity Consumption (KWh/ GGE)	7.2
Gasification & Reforming Steam (lb / GGE)	20.5
Water Consumption (Gal Water / GGE)	2.8
Carbon Conversion Efficiency (C in Fuel/C in Feedstock)	27.95%

Feedstock Rate and Cost

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).xlsm

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1 Introduction

This report documents the 2021 state of technology (SOT) assessment for the conversion of lignocellulosic biomass to high-octane gasoline (HOG) through indirect liquefaction (IDL) to syngas and methanol (MeOH) and dimethyl ether (DME) intermediates. The assessment is based on the conceptual process model for the IDL HOG pathway published in the 2015 design report (Tan et al. 2015). In the fiscal year 2020 (FY20) SOT assessment, the Aspen Plus process model underwent a significant rebuild to better support integration of new experimental data sets, reduce computational time, improve separations strategies, and improve heat integration and recycle optimization. Also, in the FY20 SOT, several isobutane (iC4)-to-DME feed ratios were experimentally simulated to determine an optimized reactor feed condition. This earlier study found that the iC4/DME molar ratio = 1.2 was the most favorable of the studied cases and was selected as the FY20 SOT base case. To maintain consistency, the FY21 SOT also utilized the rebuilt Aspen Plus model framework, and the assessment is based on updated experimental data with a base case data set (iC4/DME molar ratio = 1.2).

The focus of this assessment is the experimental and process modeling updates since the FY20 SOT report (Harris et al. 2021). In FY21, experimental efforts focused on quantifying the selectivity of aromatic compounds during hydrocarbon synthesis. To do so, the DME homologation reaction was performed at a sufficient scale (220 g catalyst loading) for liquid product collection, and a thorough analysis of the liquid hydrocarbon product was conducted to accurately quantify the aromatic content. Additionally, the mass balance closure was determined from direct mass measurements of reactants and products and was found to be within 6.5% of closure. The scale of operation used here in FY21 represents our largest amount of Cu/BEA catalyst tested in the laboratory environment to date. The operation of a continuous distillation unit for product separation and condensation is also novel in this work. Research performed in FY19–FY21 identified that less-severe regeneration temperatures are required for the National Renewable Energy Laboratory's (NREL's) Cu/BEA catalyst compared to typical zeolite catalysts. Cu-based catalysts, like those used commercially in methanol synthesis, exhibit lifetimes up to 5 years, and slow sintering and sulfur poisoning are the largest contributors to catalyst deactivation (Bartholomew and Farrauto 2005). Reduced regeneration temperatures for the Cu/BEA catalyst and sulfur-removal steps early in the conversion process promote favorable conditions for prolonged catalyst lifetime. Additionally, recent characterization work of regenerated post-reaction Cu/BEA catalysts has not found any evidence of sintering or particle agglomeration (Wu et al. 2021). As such, the lifetime of the Cu/BEA zeolite was increased to match that of the Cu-based methanol synthesis catalyst in this assessment from 2 years to 3 years. Catalyst lifetime improvements reduced operating expenses, leading to cost reductions which helped achieve FY21 cost targets. The majority of the Aspen Plus process model remained unchanged from the previous FY20 SOT. However, discussions with an engineering consulting firm identified room for process improvement by reducing the excess air requirement in combustors from a 20% stoichiometric excess to 10%. Although we limit adjustments to process and operating conditions during our year-to-year SOT assessments to avoid changes in the basis, legitimate adjustments and corrections such as these are made. For example, we made adjustments to increase the syngas pressure drop in FY20, which had a negative economic impact on the FY20 SOT assessment. The culmination of these experimental results and process modifications were used to complete the techno-economic assessment detailed in this report.

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

2 Process Description and Assumptions

A simplified process flow diagram of the 2021 SOT model is shown in Figure 1. The overall process design features five major processing steps: (1) indirect gasification of biomass, (2) syngas cleanup and conditioning, (3) catalytic conversion of syngas to methanol, (4) methanol dehydration to DME, and (5) 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 (Tan et al. 2015; Harris et al. 2021; Tan et al. 2020; Dutta et al. 2011). Syngas to methanol (step 3) and methanol dehydration to DME (step 4) are based on commercially operated processes. The bulk of the advancements and process modifications in this report were related to developments in the conversion of DME to branched hydrocarbons. Advancements included increased single-pass DME conversion, increased C_5+ product selectivity, and decreased aromatics production. The details of these changes are outlined later in this report.
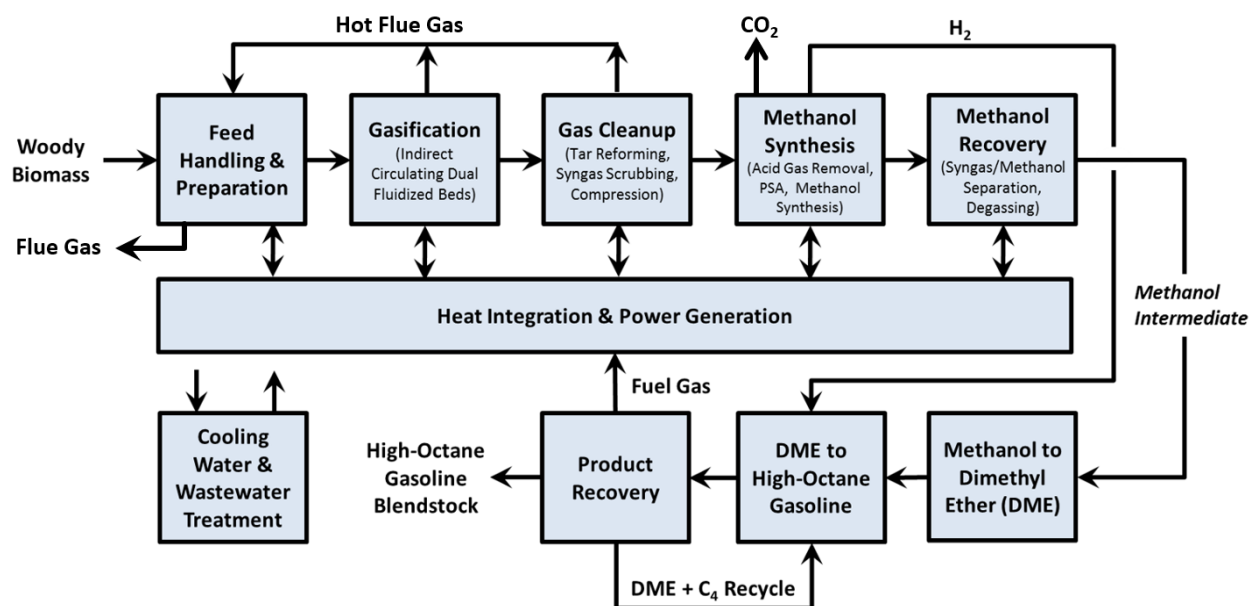
Figure 1. Process flow diagram for the production of high-octane gasoline blendstock via syngas conversion pathway and methanol/dimethyl ether intermediates

PSA = pressure swing adsorption

3 Feedstock Specifications and Costs

The 2021 IDL SOT feedstock composition and cost information used in this analysis was provided by Idaho National Laboratory and is described in detail in their *Woody Feedstocks 2020 State of Technology Report* (Hartley, Thompson, and Cai 2020). Overall, feedstock specifications remained consistent with those reported in both the 2019 and 2020 IDL SOT reports (Harris et al. 2021; Tan et al. 2020). The delivered feedstock cost was calculated by Idaho National Laboratory 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 2021 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] (British thermal unit [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

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4 Financial Assumptions for Techno-Economic Analysis

The techno-economic analysis (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. A minimum fuel selling price (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 (Tan et al. 2015). A summary of the assumptions applied in this report is listed in Table 2.

Table 2. Summary of nth-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 2021 SOT

5.1 Experiment and Results

Pre-oxidized 10 wt % Cu/BEA catalyst extrudate pellets (221.4 g) were loaded into a series of four stainless-steel reactors positioned in series with one another. Reactor temperature was controlled via shell-and-tube heat exchange (i.e., oil-jacketed) reactor tubes. The total catalyst bed volume was 430 mL. Within each reactor tube, a four-point thermocouple was positioned within the isothermal oil-jacketed catalyst bed and was used to monitor reaction temperature. The reaction temperature was maintained within ±2.5°C of the nominal reaction set point (230.5°C) across all reactor thermocouple points. Prior to this experiment, this same catalyst loading had been used for 287 h of time-on-stream DME homologation experimentation, under reaction conditions nearly identical to those described below. The catalyst bed from the original experiment remained in place here, unmanipulated other than a reduction with H_2 prior to starting the experiment. The pretreatment procedure for the original experiment was identical to the following description of the reduction procedure used for this experiment.

The catalyst was reduced in flowing H_2 at 1.5 L-min^{-1} for at least 4 h at 250°C (approximately 2°C/min ramp rate) before cooling to 200°C. The catalyst was then exposed to the reaction mixture, and product sampling began. DME was fed to the reactor as a liquid at 5.2 MPa and was vaporized through an orifice and allowed to equilibrate to reactor system pressure (120–360 kPa). The mass flow of DME and 95% H_2/Ar into the reactor system were measured directly and independently with a Coriolis meter to provide g-h^{-1} (Bronkhorst, M12). The reaction was started at 120 kPa absolute and 200°C. The reactor temperature and system pressure were incrementally increased simultaneously (5°C and 30–70-kPa increments), with at least a 1-h hold at each step, until final stable reactor conditions were achieved. Final experimental conditions were 230.5°C ± 2.5°C, a system pressure of 360 kPa, and a DME space velocity (SV) of 0.4 g_{DME}-g_{cat}^{-1}-h^{-1} (referred to as h^{-1}). The H_2-to-DME molar ratio was maintained at 1.1:1.0 H_2 to DME.

System plugging due to condensation and/or freezing of the byproduct hexamethylbenzene (HMB) has plagued prior attempts for long-term operation of the DME homologation chemistry at greater than 10 g catalyst loading. To prevent this, an aromatic solvent was introduced (C_{11}–C_{15} methylated aromatics; 10.3 g-h^{-1}) to the reactor effluent, prior to the fluid stream entering the distillation column. The distillation column (90-cm height) was operated at the same pressure as the reactor (360 kPa). Liquid samples accumulated in the reboiler vessel and were drained periodically, weighed for mass measurement, and saved for analysis. A liquid inventory was maintained in the reboiler to prevent excess system pressure perturbations and excess gaseous product from entering the final collection vessel. Non-condensed products exited the top of the distillation column (i.e., tailgas), and the mass flow rate of this stream was measured by a third and final Coriolis meter. The tailgas fluid was 0.5°C ± 0.5°C as it exited the distillation column, and the reboiler fluid was kept at 92.5°C ± 2.5°C. The entire length of the distillation column was filled with inert stainless-steel perforated column packing (Cannon, Pro-Pak). The design of the distillation column was performed with isobutane as the "light key" species and 2,2,3-trimethyl-butane (triptane) as the "heavy key" species, such that isobutane was intended to leave the system in the tailgas stream and triptane was intended to be removed in the liquid samples (along with HMB and the aromatic solvent).

Table 3. Summary of 2021 Experimental Performance Relative to Major Technical Targets

Process Parameter	2021 Target	2021 SOT [a]	2022 Projection
Hydrocarbon synthesis reactor temperature	225°C	230°C	225°C
Single-pass DME conversion	39.7%	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	83.4% (overall)	76.0% (single-pass)	86.7% (overall)
Carbon selectivity to aromatics	2.4% aromatics (1.4% HMB)	1.6% HMB only	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% iC4 recycle efficiency [b] at iC4/DME ratio of 1.2	Recycled to hydrocarbon synthesis reactor: 40% recycle efficiency

[a] Total mass balance, excluding contribution from co-fed aromatic solvent, closed to within 6.5% of ideal

[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 Mass Balance and Aromatics Quantification

Reactor inlet and outlet, as well as the tailgas effluent from the distillation column, were sampled through heated (220°C) lines with an Agilent 7890 gas chromatography (GC) instrument equipped with a flame ionization detector for analysis of oxygenates and hydrocarbons and two thermal conductivity detectors for analysis of permanent gases. GC responses for reactants and products were calibrated using traceable gravimetric gas standards. Ar was used as the internal standard for gas chromatography. Catalyst performance was evaluated, in part, from inlet flow and GC measurements using Ar as an internal standard. The conversion, X (in carbon %), was calculated according to Equation 1 based on inlet and effluent DME molar flow rate:

$$X = \frac{\dot{n}_{DME,in} - \dot{n}_{DME,out}}{\dot{n}_{DME,in}} \tag{1}$$

where $\dot{n}_{DME,in}$ and $\dot{n}_{DME,\,out}$ represent molar flow rates (mol-s^{-1}) in DME, and $\dot{n}_{DME,\,out}$ was taken at the effluent of the reactor. To allow for adequate liquid sample, the mass balance period consisted of 14 h of time on stream. The deviation from mass balance closure over that time period was calculated according to Equation 2:

$$Mass\ Balance = \frac{m_{DME} + m_{95H2} - m_{tailgas} - m_{liq\ formed} - m_{GC\ sampling}}{m_{DME} + m_{95H2}} \tag{2}$$

where m_{DME} is the cumulative mass of DME fed to the reactor as measured by the Coriolis meter, m_{95H2} is the cumulative mass of 95% H_2/Ar fed to the reactor as measured by the Coriolis meter, $m_{tailgas}$ is the cumulative mass of the distillation effluent gaseous stream, $m_{liq\ formed}$ is the total net mass of the liquids formed from reaction (i.e., total liquid sample less mass of aromatic solvent fed) as collected from the collection vessel, and $m_{GC\ sampling}$ is the mass lost to the online gas

6

chromatography during the collection period (gas flow to GC constant) as calculated from compositional analysis data and a volumetric flow rate. All values are in grams and were taken over the 14-h mass balance collection period. The influence of the mass of the aromatic solvent was intentionally neglected in this calculation, as the solvent was not involved in the DME homologation reaction, and quantification of solvent mass was facile and tended to artificially improve the metric.

The HMB and all other liquid hydrocarbon species were quantified with GC-vacuum ultraviolet spectroscopy (VUV) to provide a PIONA weight percent distribution (i.e., n-paraffin, isoparaffin, olefin, naphthenes, and aromatics for C_1–C_{19} hydrocarbons). The carbon selectivity to HMB was calculated according to Equation 3:

$$S_{C,HMB} = \frac{\dot{n}_{C,HMB}}{\sum \dot{n}_{C,products}} \tag{3}$$

where $\dot{n}_{C,HMB}$ and $\dot{n}_{C,\,products}$ are the flow of carbon in HMB and all products, respectively, in mol_C-h^{-1}. For comparison to prior data and due to incomplete species identification from GC-VUV, the molar flow rates for $\dot{n}_{C,\,products}$ were calculated from online gas-phase GC analysis at the reactor effluent. The $\dot{n}_{C,\,HMB}$ is calculated according to Equation 4:

$$\dot{n}_{C,HMB} = \dot{n}_{C,triptane} * \frac{m_{C,HMB}}{m_{C,triptane}} \tag{4}$$

where $\dot{n}_{C,triptane}$ is the molar carbon flow in triptane, in mol_C-h^{-1}, from gas-phase GC analysis at the reactor effluent. $m_{C,triptane}$ and $m_{C,HMB}$ are the mass of carbon in triptane and HMB, respectively, in the organic phase of the liquid sample. Both values were calculated simply as mass of the organic phase multiplied by weight percent concentration from GC-VUV. Effectively, Equations 3 and 4 calculate the carbon selectivity to HMB by using the carbon mass ratio of HMB to triptane in the collected organic phase liquids, and the molar flow rates for all other products from gas-phase GC analysis at the reactor effluent. The collection of liquid samples and use of an analytical technique that was able to quantify HMB allowed this reactor system to provide accurate quantification of HMB not otherwise achievable by gas-phase GC analysis alone.

5.1.2 Model Assumptions and Inputs

The carbon and species selectivity metrics included in the FY21 SOT assessment are consistent with the findings in the FY20 SOT assessment. In FY20, several iC4/DME ratios were investigated experimentally to determine the reactor feed conditions that resulted in optimized DME-to-HOG conversion metrics. This previous analysis determined the iC4/DME ratio equal to 1.2 yielded favorable single-pass DME conversion and C_5+ product selectivity, and thus was chosen as the base SOT case for FY20. The same ratio case was selected as the basis for the FY21 SOT; however, new analytical results determined aromatics formation was reduced from a total of 3.3% (FY20) to 1.6% (FY21), with 100% species selectivity to HMB (i.e., no additional aromatic species were detected in collected liquid samples). Therefore, the modeled carbon selectivity to aromatics was reduced based on most recent experimental values with the updated aromatics content, and the remainder of the carbon species were renormalized for the model input. Experimental efforts towards complete mass and carbon balance closures to reduce uncertainties in assumptions will be an area of focus in future years. A detailed summary of carbon selectivity and species selectivity utilized in this assessment are reported in Table 4. Additionally, research exploring the regeneration conditions required for NREL's Cu/BEA catalyst determined that less-severe conditions are sufficient for catalyst

reactivation (Wu et al. 2021). Together with low aromatics formation, the Cu/BEA catalyst lifetime was extended in the FY21 assessment from 2 years to 3 years to match that of the Cu-based methanol synthesis catalyst.

Table 4. 2021 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
C_1	1.78%	Methane (CH_4)	100.00%
C_2	1.19%	Ethane (C_2H_6)	14.47%
		Ethene (C_2H_4)	85.53%
C_3	2.00%	Propane (C_3H_8)	33.84%
		Propene (C_3H_6)	66.16%
C_4	20.09%	Methylpropane (C_4H_{10})	89.12%
		n-Butane (C_4H_{10})	3.59%
		2-Methylpropene (C_4H_8)	2.83%
		But-1-ene (C_4H_8)	4.46%
C_5	23.40%	2-Methylbutane (C_5H_{12})	97.31%
		2-Methylbutene (C_5H_{10})	2.69%
C_6	6.25%	3-Methylpentane (C_6H_{14})	31.19%
		2,3-Dimethylbutane (C_6H_{14})	60.73%
		2,3-Dimethylbutene (C_6H_{12})	8.08%
C_7	22.09%	2,2,3-Trimethylbutane (C_7H_{16})	45.59%
		2,4-Dimethylpentane (C_7H_{16})	26.19%
		2-Methylhexane (C_7H_{16})	22.62%
		2,2,3-Trimethylbutene (C_7H_{14})	0.30%
		2-Methyl-1-Hexene (C_7H_{14})	5.31%
C_8	8.18%	2,2,4-Trimethylpentane (C_8H_{18})	89.48%
		2,4,4-Trimethyl-1-pentene (C_8H_{16})	10.52%
C_8 + cyclic	10.40%	Dimethylcyclohexane (C_8H_{16})	24.12%
		Trimethylcyclohexane (C_9H_{18})	75.88%
C_9+	3.02%	Trimethylpentane (C_9H_{20})	100.00%
Aromatics (HMB)	1.60%	Hexamethylbenzene ($C_6(CH_3)_6$)	100.00%
Aromatics (Others)	0.00%	Methylbenzene (C_7H_8) [a]	0.00%
Total	**100%**		

[a] Model compound representing other aromatics.

This report is available at no cost from the National Renewable Energy Laboratory (NREL) at www.nrel.gov/publications.

5.2 Techno-Economic Analysis Results

Experiments conducted in support of achieving the FY21 MFSP cost target of $3.40 per gallon of gasoline equivalent (GGE) included a decrease in overall aromatics formation from 3.3% in FY20 to 1.6% in FY21. Further, recent research into the regeneration of the Cu/BEA catalyst demonstrated a lower temperature requirement than typical zeolite catalysts, indicating that the overall lifetime of the catalyst resembles that of robust Cu catalysts rather than more sensitive zeolites. As such, the lifetime of the Cu/BEA catalyst was increased from 2 years to 3 years for the FY21 assessment. Additionally, with new engineering guidance from an engineering firm, the modeled amount of excess air fed to process combustors was reduced from the original assumption of 20% to 10% excess based on the stoichiometric requirement of oxygen. All three of these modifications were applied to determine the FY21 SOT base case MFSP of $3.38/GGE, surpassing the FY21 target. A summary of key performance metrics for the FY21 SOT and the 2022 projection case are included in Table 5.

The total HOG production in the 2021 SOT is 51.7 GGE per dry U.S. ton of feedstock, a slight increase of 0.3 GGE from the previous 2020 SOT. No liquid petroleum gas (LPG) is recovered in the FY21 SOT, in line with the overall goal of high C_5+ fuel yields. Overall annual operating costs and capital costs in the FY21 SOT are approaching those targeted in the FY22 projection, at $76 million annually and $407 million, respectively. Reduced aromatic formation increases HOG range product selectivity; however, higher selectivity toward highly branched hydrocarbons versus aromatic compounds results in slightly greater hydrogen consumption in the DME-to-HOG step based on the reaction stoichiometry. Thus, the net yield increases and MFSP decreases from aromatic reduction alone were negligible. However, reduced aromatic formation is also an important factor for catalyst longevity. This, in combination with regeneration research efforts, supports the modification to a 3-year Cu/BEA lifetime in the FY21 SOT versus 2-year lifetime in previous analyses. The improved catalyst lifetime reduces operating expenses and resulted in approximately a $0.05/GGE cost reduction. Finally, reducing excess air to the process combustors had the two-fold effect by lowering energy consumption of combustion air blowers and reducing the volume of material into the combustors, decreasing associated capital expenses. This process modification resulted in about a $0.03/GGE cost reduction.

Table 5. Summary of Process Performance and Economic Results

	2021 SOT	2022 Projection
Feedstock rate	2,205 dry U.S. tons/day	
Online time	7,884 h/yr (90% online factor)	
Total C$_5$+ fuel yield	51.7 GGE per dry U.S. ton feedstock	54.7 GGE per dry U.S. ton feedstock
LPG coproduct	—	—
Total fuel production rate C$_5$+ [LPG]	37.5 [0] million GGE per year	39.6 [0] million GGE per year
Total annual operation cost and credits	$76 million	$79 million
Total installed equipment cost	$234 million	$228 million
Total capital investment	$407 million	$397 million
Total capital investment per annual gallon	$10.85/GGE	$10.03/GGE
Minimum fuel selling price	**$3.38/GGE**	**$3.30/GGE**
Feedstock costs	$1.22/GGE	$1.11/GGE
Operating costs and credits	$0.80/GGE	$0.66/GGE
Capital charges and taxes	$1.35/GGE	$1.54/GGE

A cost breakdown for the major processing areas in the IDL pathways is provided in Figure 2. The largest contributor, per the breakdown provided below, is the feedstock cost, which contributes 36.5% ($1.23/GGE) of the total costs. The syngas cleanup and compression step contribute the next largest percentage at about 27.3% ($0.92/GGE) of the total MFSP. The conversion of MeOH to DME, DME to HOG, and the HOG separations step together amount to about $0.40/GGE, or 11.7%. Increasing the Cu/BEA catalyst lifetime from 2 years to 3 years reduced the cost of DME conversion to HOG from $0.28/GGE to $0.23/GGE. Consistent with previous SOT cases, combustion of process off-gases and a small percentage of raw syngas generates steam for a combined heat and power system, and thus no external natural gas or electricity is purchased in this process design. The quantity of syngas used for heat and power generation is manipulated such that electricity generation and consumption at the plant sum to near zero. To supply hydrogen to the DME-to-HOG reactor, pressure swing adsorption is used to extract hydrogen from syngas in the MeOH synthesis area, and therefore no external hydrogen is imported. Per the 2020 SOT assessment and in accordance with 2022 process projections, no LPG is recovered for coproduct credit (Harris et al. 2021). Butanes and lighter gases are either recycled to the DME-to-HOG reactor for iC4 reactivation to increase HOG yields or directed to the tar reformer combustor for process heat and power.
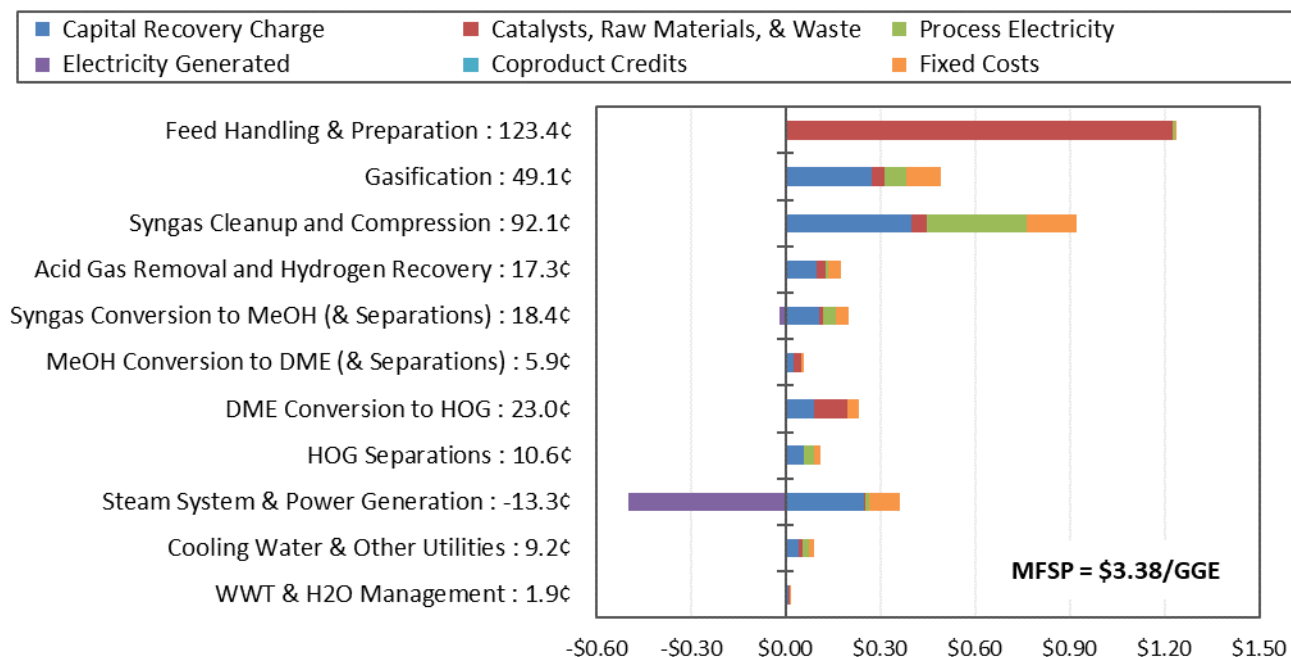
Figure 2. Cost breakdown for the 2021 SOT model

WWT = wastewater treatment

5.3 Sensitivity Analysis

A sensitivity assessment was performed on the FY21 SOT baseline case to determine key process drivers, understand the impact of uncertainty, and identify target metrics for future analyses. Figure 3 shows a summary of the sensitivity cases as a percent change from the baseline MFSP of $3.38/GGE. The assessment evaluated financial and process parameters to gauge the impact of both market changes and technical variations.

Case 1 shows the impact of varying IRR on the 40% equity (Table 2). In a scenario with an IRR of 0%, the MFSP decreased by 25.9% ($2.50/GGE); increasing the IRR from the baseline value of 10% to 20% resulted in an MFSP increase of 27.7% ($4.31/GGE). Other financial parameters that resulted in significant variation from the baseline case included total capital investment (Case 2) and average installation factor (Case 3). A 10% decrease to either variable led to a corresponding 5% decrease in MFSP ($3.21/GGE). Likewise, an increase of 30% in either variable resulted in a 14.9% increase in MFSP ($3.88/GGE). As discussed in Section 5.2, the feedstock contributes about 37% of the total costs, and therefore the final MFSP is sensitive to feedstock purchase cost. A 20% increase or decrease in feedstock cost resulted in a $0.25/GGE (7.3%) increase or decrease in the MFSP, respectively. Other financing parameters, including steam turbine capital cost (Case 15), equity versus debt financing (Case 16), and acid gas removal capital cost (Case 17), result in only small changes to the MFSP.

In the FY20 SOT assessment, a new sensitivity scenario was introduced investigating the potential of obtaining credit for CO_2 capture and sequestration under the 45Q tax credit (Harris et al. 2021; Carbon Capture Coalition 2021; Christensen 2019). An acid gas removal unit is necessary in the current process design to reduce the CO_2 concentration in the methanol synthesis reactor feed stream down to 5% by volume for optimal operation. The high-purity CO_2 stream from the acid gas

removal, which is currently released to the atmosphere, meets the eligibility requirements for a maximum credit of $50/ton CO_2. Because the CO_2 from the acid gas removal unit would require additional compression and final purification costs that were not modeled in this assessment, the maximum credit value was limited to $40/ton CO_2 for this sensitivity case. Case 4 in Figure 3 shows that applying the $40/ton credit resulted in an MFSP reduction of 9.7%, or an MFSP value of $3.05/GGE.

Several sensitivity cases were also performed around key process variables, including hydrocarbon synthesis catalyst lifetime, C_5+ hydrocarbon yield, excess air to combustors, and aromatics selectivity. Hydrocarbon synthesis catalyst (Cu/BEA) lifetime was a key process variable modified in the FY21 SOT assessment. Case 8 looked at a catalyst lifetime of 5 years and 1 year, which resulted in MFSPs of $3.34/GGE and $3.58/GGE, respectively. In this year's assessment, the quantity of excess air to the combustors was reduced from 20% stoichiometric excess to 10%. This resulted in an overall MFSP reduction of $0.03/GGE, or a 0.8% reduction as shown in Case 19. Varying the aromatics selectivity (Case 20) from the baseline value of 1.6% (HMB only) to 1.0% resulted in an MFSP of $3.36/GGE. Conversely, an increased aromatic selectivity to 3.0% resulted in an increased MFSP of $3.40/GGE.

Case 10 addresses uncertainty associated with mass balance closure of experimental data sets, which is assumed here to impact the C_5+ hydrocarbon selectivity (base case = 73.3%). Recent experiments closed the total mass balance to within 6.5%. Improvements in experimentally demonstrated mass balance closure are expected in subsequent years; however, the resultant effect on C_5+ hydrocarbon selectivity is not fully quantified. As a means of estimating the impact of mass balance improvement on MFSP, two high-level scenarios are proposed for this case to bracket the possible results: a high C_5+ hydrocarbon yield in which the 6.5% mass unaccounted for is assumed to be C_5+ hydrocarbons, and a low-yield scenario in which the mass is assigned to C_4 or lower hydrocarbons, providing C_5+ selectivity values of 75.0% and 68.6%, respectively. The MFSP was reduced by 1.6% ($3.32/GGE) and increased by 5.0% ($3.55/GGE) for the high and low C_5+ hydrocarbon yield sensitivities, respectively. Future experimental efforts will be conducted to reduce uncertainty in mass balance closure.
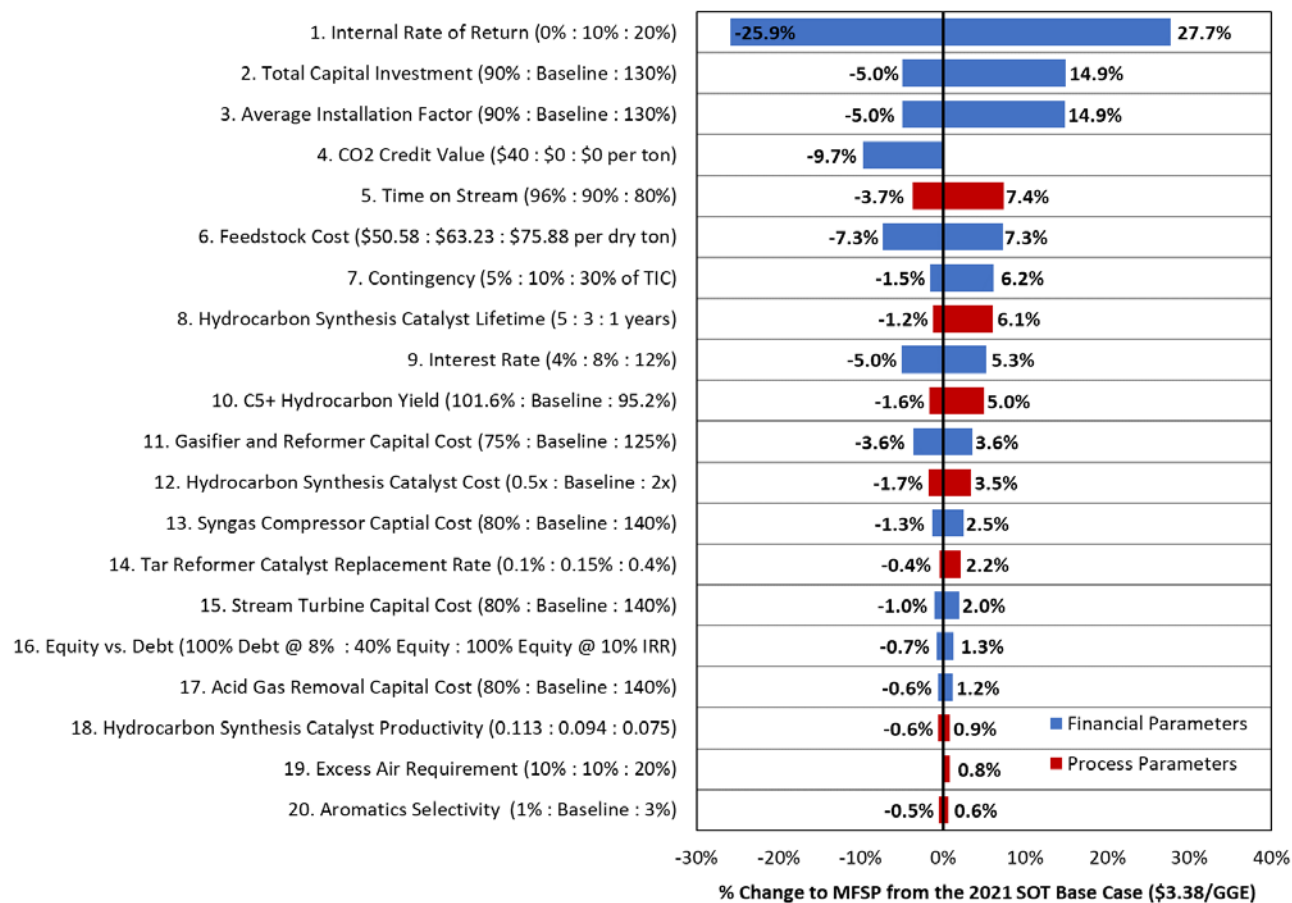
Figure 3. Sensitivity analysis for the 2021 SOT base case

6 Sustainability Assessment

A sustainability assessment was carried out as part of the FY21 SOT analysis. Table 6 summarizes the material and energy flows obtained from the Aspen Plus model and utilized for the sustainability assessment. The material flows include the products, consumed resources, wastes, and direct air emissions from the proposed biorefinery. The 2021 SOT only produces a high-octane gasoline fuel product, as the LPG coproduct was eliminated in the FY20 assessment (Harris et al. 2021). Additionally, combustion of syngas and process off-gases are balanced such that a negligible amount of electricity is imported or exported, and no external heat sources are required. Biogenic CO_2 air emissions are split into two categories to delineate the fraction of CO_2 in flue gas and the fraction of concentrated CO_2 from the acid-gas removal system available for potential sequestration. The material and energy flows compiled in Table 6 for a conversion process lifecycle inventory and will be further incorporated by Argonne National Laboratory for a full supply chain sustainability assessment.

Table 6. Material and Energy Flows for the HOG Conversion Process (Gate-to-Gate)

Cases		2021 SOT	2022 Projection
		Production Rate	**Production Rate**
Products			
HOG	lb/h	28,961	30,768
	gal/h	5,105	5,144
	million Btu/h	552	583
HOG properties	LHV (Btu/gal)	108,029	113,309
	Density (g/gal)	2,573	2,713
	Biogenic C in HOG, %	100.0%	100.0%
	C content in HOG, wt %	83.8%	83.1%
Byproducts			
Mixed butanes (LPG)	lb/h	—	—
	gal/h	—	—
	million Btu/h	—	—
LPG properties	LHV (Btu/gal)	—	—
	Density (g/gal)	—	—
	Biogenic C in HOG, %	—	—
	C Content in HOG, wt %	—	—
Sulfur	lb/h	116	114
Excess electricity	hp	4	(36)
Resource Consumption		**Flow Rate (lb/h)**	**Flow Rate (lb/h)**
Blended woody biomass (wet)		262,455	262,455
Blended woody biomass (dry)		183,718	183,718
Magnesium oxide (MgO)		13	23
Fresh olivine		539	527
Tar reformer catalyst		10	9
Natural gas for reformer		0	0

Cases	2021 SOT	2022 Projection
Methanol synthesis catalyst	5	5
DME catalyst	9	6
Beta zeolite catalyst	26	34
Zinc oxide catalyst	2.5	2.5
Shift catalyst	0.2	0
Cooling tower water makeup	54,481	31,213
Boiler feedwater makeup	10,108	86,887
Other freshwater makeup [a]	64,421	0
Dimethyl disulfide (DMDS)	2.1	2.1
Amine (MDEA) makeup	4.3	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	69
Waste Streams	**lb/h**	**lb/h**
Sand and ash purge	4,129	6,679
Tar reformer catalyst	8.8	8.7
Scrubber solids	116	8.8
Wastewater	2,540	14,845
Air Emissions	**lb/h**	**lb/h**
CO_2 (biogenic – flue gas)	168,598	174,957
CO_2 (biogenic – concentrated, potential sequestration)	77,944	66,887
CO_2 (fossil)	0	0
CH_4	0	0
CO	0	0
NO_2	70	142
SO_2	49	51
H_2O	135,668	73,422
H_2S	0.6	0
Heating Values of Fuel to Combustors	**million Btu/h**	**million Btu/h**
Char combustor		
LHV to char combustor	430	528
HHV to char combustor	447	553
Char combustor % biogenic C	100%	100%
Fuel combustor		
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 the 2021 case.

A summary of the sustainability metric indicators for the IDL pathway is given in Table 7. In addition to the results from the 2021 SOT, the 2020 SOT and the 2022 projection results are also provided for reference. The HOG yield in the FY21 SOT is slighter greater than the FY20 SOT at 51.7 GGE/dry U.S. ton of biomass feedstock; however, this remains below the 2022 projection. Improvements in future C_5+ product selectivity, such as via further recycled iC4 incorporation into liquid-range products, may help achieve the 2022 target of 54.7 GGE/dry U.S. ton of biomass. In all three cases, the LPG coproduct has been eliminated. Butanes are recycled to the DME-to-HOG reactor to help improve conversion to HOG-range products, and excess butanes and lighter gases are recycled to the reformer to produce more syngas or combusted for process heat and power. Because this process uses internal off-gases and syngas for heat and power, electricity and natural gas imports are negligible. Water consumption in the FY21 SOT case remained consistent with the FY20 SOT case at 3.3 gal/GGE, slightly above the 2022 projection. ANL calculated supply chain GHG emissions for the FY21 SOT case of 18 g CO_2e/MJ. Thus, like both the FY20 SOT and FY22 projection, the FY21 SOT, with a computed reduction of 80%, exceeded our supply chain GHG emission reductions target of >60% relative to the fossil baseline.

Table 7. Summary of Sustainability Metric Indicators for the 2020 SOT, 2021 SOT, and 2022 Projection Cases

Sustainability Metrics	Units	2020 SOT	2021 SOT	2022 Projection
HOG fuel yield by weight of biomass	GGE per dry U.S. ton biomass	51.4	51.7	54.7
LPG fuel yield by weight of biomass	GGE per dry U.S. ton biomass	—	—	—
Carbon efficiency to HOG + LPG	% C in feedstock	26 + 0	26.2 + 0	28 + 0
Electricity import	kWh/GGE	—[a]	—[a]	—[a]
Natural gas import	MJ/GGE	—[b]	—[b]	—[b]
Water consumption	gal/GGE	3.3	3.3	2.8
Water consumption	m^3/day	1,406	1,409	1,286

[a] Negligible

[b] No natural gas import

7 Conclusions

The FY21 SOT report outlined the updates and achievements for the indirect liquefaction of biomass to high-octane gasoline pathway. Since the FY20 SOT, a rigorous quantification technique for aromatics selectivity was developed. This resulted in a calculated aromatics selectivity lower than previous projections at 1.60% (HMB only). Reduced aromatics formation is favorable from an operational standpoint as the reduction of coke precursors reduces the potential for catalyst fouling, and reduced aromatics allows more carbon to be favorably converted to non-aromatic hydrocarbon products. Additional research conducted over the last few years found that NREL's Cu/BEA zeolite requires lower temperatures for regeneration, which favorably impacts catalyst longevity. Also, in the FY21 SOT assessment, updated assumptions surrounding the excess air requirement of process

combustors were incorporated into the Aspen Plus process model. Per recommendations from an engineering firm, air was reduced from a 20% stoichiometric excess to 10%, reducing both operating and capital expenses for those unit operations. Together, these developments resulted in a modeled MFSP of $3.38/GGE, less than the projected 2021 target of $3.40/GGE.

8 Future Work

Future work will build on the learnings generated in the FY21 SOT assessment, while also redirecting research efforts from the traditional three-step conversion of syngas to HOG through MeOH and DME intermediates, to a single-step syngas-to-hydrocarbons (STH) approach. A high-level depiction of this approach is shown in Figure 4.
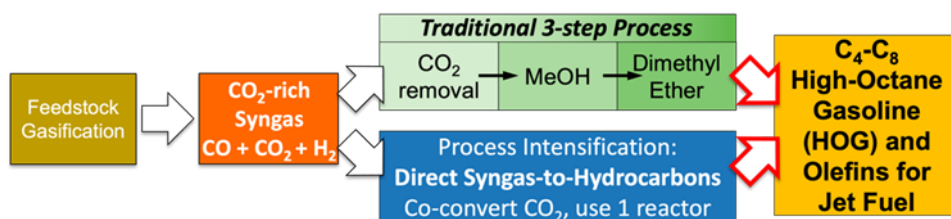
Figure 4. Schematic comparing the traditional three-step process and the STH process intensification approach for hydrocarbon production from biomass syngas

The direct conversion of syngas to hydrocarbons in a single reactor using commercial syngas-to-DME catalysts and NREL's Cu/BEA DME-to-hydrocarbons catalyst is a nascent approach that began in FY20. Initial exploratory research found that this pathway is highlighted by high CO conversion, high C_4+ product selectivity, and co-fed CO_2 activation and incorporation into hydrocarbon products. The STH pathway also holds great potential as a commercially viable, economically competitive route to sustainable aviation fuels (SAF). The high selectivity to C_4+ hydrocarbons with minimal aromatics results in approximately 95% of hydrocarbon products as sustainable aviation fuel precursors. Downstream dehydrogenation and coupling of the C_4+ hydrocarbons are known industrial processes. The advantages of direct STH over the three-step process are the potential reduction in number of unit operations (fewer reactors and intermediate separation steps) and reduction in separations intensity (higher pressure allows for product condensation near ambient temperatures), resulting in reduced capital and operating expenses. Compared to the three-step process, where DME handling presents an operational challenge due to the physical properties of this low-boiling-point reactant, the STH pathway offers greater operational flexibility for technology advancement. Overall, higher-pressure operation can be achieved with syngas feeds instead of DME, and this is anticipated to facilitate improved product recovery and smaller equipment size by volume, reducing capital expenses and improving MFSP.

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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 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%

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)	($0.36)
Sustainability and Process Efficiency Metrics										
Carbon Efficiency to C_5+ Product	% C in Feedstock	19.3%	19.4%	25.2%	24.3%	25.5%	24.8%	26.1%	26.2%	27.9%
Carbon Efficiency to Mixed C_4 Co-Product	% C in Feedstock	7.0%	6.9%	0.0%	0.0%	0.0%	2.3%	0.0%	0.0%	0.0%
Overall Carbon Efficiency to Hydrocarbon Products	% C in Feedstock	26.3%	26.3%	25.2%	24.3%	25.5%	27.1%	26.1%	26.2%	27.9%
Overall Energy Efficiency to Hydrocarbon Products	% LHV of Feedstock	37.7%	37.7%	36.6%	35.1%	36.6%	39.6%	37.6%	37.9%	40.4%
Electricity Production	kWh / Gallon C_5+	11.7	11.8	7.9	8.4	8.1	7.6	12.2	11.9	7.0
Electricity Consumption	kWh / Gallon C_5+	11.7	11.8	7.9	8.5	8.1	7.6	12.2	11.9	7.0
Water Consumption	Gal H_2O / Gal C_5+	12.9	10.1	3.1	3.3	3.2	2.9	3.3	3.3	2.8
TEA Reference File		2014 SOT Rev4a 2016$ (high ash)_1.xlsm	2015 SOT Rev6 Comm-HBEA 2016$ FR Rev2_1.xlsm	2016 SOT Base Rev6 Rev2 2016$ FR_1.xlsm	2017 SOT Base Rev1 2016$ FR_1 KH (Feedstock Cost).xlsm	2018SOT_2018-07-20data Rev3_2 KH (Feedstock Cost).xlsm	2019 SOT Oct Update Rev02 - (C4-DME-1_LPG) Rev0_b.xlsm	HOG2020-V117_rev5.xlsm	HOG2021-V006b-air excess red_3yr.xlsm	2022 Design FR Rev5a_2 KH (Feedstock Cost).xlsm

▲ Conceptual design result

† SOT: state of technology.

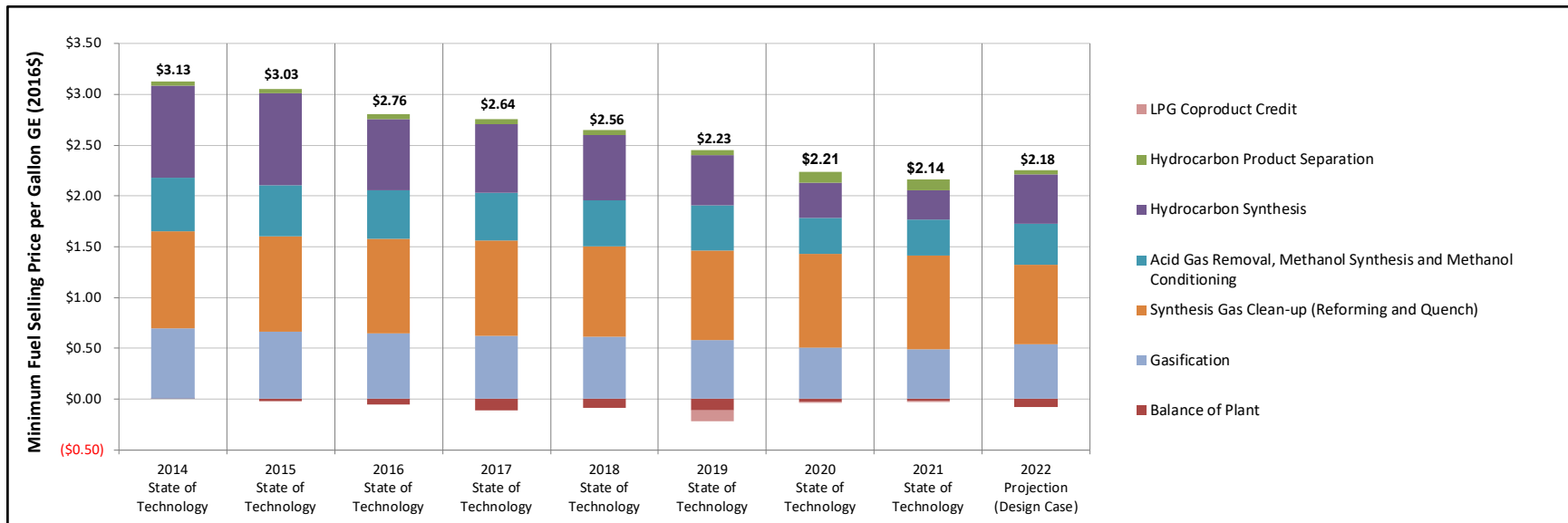| Minimum Fuel Selling Price (MFSP) Breakdown ($ / Gallon of Gasoline Equivalent)	2014 State of Technology	2015 State of Technology	2016 State of Technology	2017 State of Technology	2018 State of Technology	2019 State of Technology	2020 State of Technology	2021 State of Technology	2022 Projection (Design Case)
Gasification	$ 0.69	$ 0.67	$ 0.65	$ 0.62	$ 0.61	$ 0.58	$ 0.50	$ 0.49	$ 0.54
Synthesis Gas Clean-up (Reforming and Quench)	$ 0.96	$ 0.93	$ 0.94	$ 0.94	$ 0.89	$ 0.88	$ 0.93	$ 0.92	$ 0.78
Acid Gas Removal, Methanol Synthesis and Methanol Conditioning	$ 0.52	$ 0.50	$ 0.47	$ 0.47	$ 0.45	$ 0.45	$ 0.36	$ 0.36	$ 0.40
Hydrocarbon Synthesis	$ 0.91	$ 0.91	$ 0.70	$ 0.67	$ 0.64	$ 0.49	$ 0.34	$ 0.29	$ 0.48
Hydrocarbon Product Separation	$ 0.04	$ 0.05	$ 0.05	$ 0.05	$ 0.05	$ 0.05	$ 0.11	$ 0.11	$ 0.05
LPG Coproduct Credit	$ -	$ -	$ -	$ -	$ -	$ (0.11)	$ (0.00)	$ (0.00)	$ -
Balance of Plant	$ 0.01	$ (0.02)	$ (0.05)	$ (0.11)	$ (0.09)	$ (0.11)	$ (0.03)	$ (0.02)	$ (0.07)
Minimum Fuel Selling Price (MFSP)	**$ 3.13**	**$ 3.03**	**$ 2.76**	**$ 2.64**	**$ 2.56**	**$ 2.23**	**$ 2.21**	**$ 2.14**	**$ 2.18**

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

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| 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 State of Technology		2022 Projection (Design Case)	
Feedstock	$	1.20	$	1.21	$	1.24	$	1.22	$	1.23	$	1.31	$	1.24	$	1.23	$	1.12
Gasification	$	0.69	$	0.67	$	0.65	$	0.62	$	0.61	$	0.58	$	0.50	$	0.49	$	0.54
Synthesis Gas Clean-up (Reforming and Quench)	$	0.96	$	0.93	$	0.94	$	0.94	$	0.89	$	0.88	$	0.93	$	0.92	$	0.78
Acid Gas Removal, Methanol Synthesis and Methanol Conditioning	$	0.52	$	0.50	$	0.47	$	0.47	$	0.45	$	0.45	$	0.36	$	0.36	$	0.40
Hydrocarbon Synthesis	$	0.91	$	0.91	$	0.70	$	0.67	$	0.64	$	0.49	$	0.34	$	0.29	$	0.48
Hydrocarbon Product Separation	$	0.04	$	0.05	$	0.05	$	0.05	$	0.05	$	0.05	$	0.11	$	0.11	$	0.05
LPG Coproduct Credit	$	-	$	-	$	-	$	-	$	-	$	(0.11)	$	(0.00)	$	(0.00)	$	-
Balance of Plant	$	0.01	$	(0.02)	$	(0.05)	$	(0.11)	$	(0.09)	$	(0.11)	$	(0.03)	$	(0.02)	$	(0.07)
Minimum Fuel Selling Price (MFSP)	**$**	**4.33**	**$**	**4.24**	**$**	**3.99**	**$**	**3.86**	**$**	**3.79**	**$**	**3.53**	**$**	**3.45**	**$**	**3.38**	**$**	**3.30**
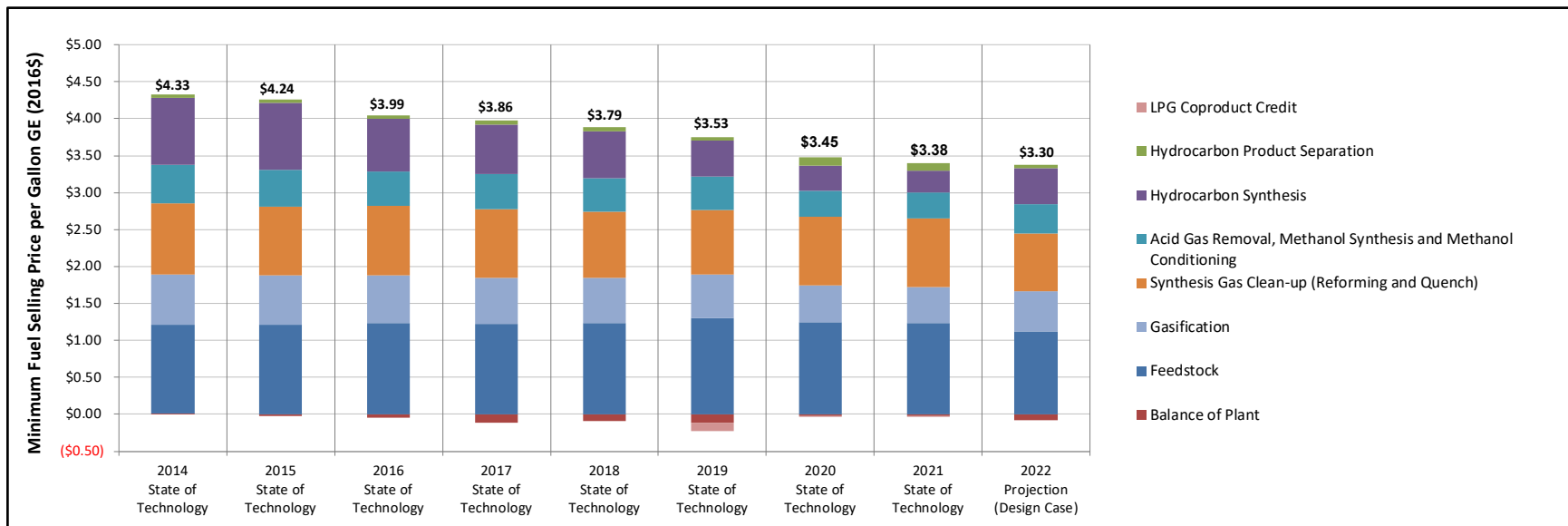
Figure A-2. SOT/waterfall for syngas conversion high-octane gasoline pathway in 2016$