



Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update

Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Pathways

Ryan Davis¹, Nicholas Grundl¹, Ling Tao¹, Mary J. Bidy¹, Eric C. D. Tan¹, Gregg T. Beckham¹, David Humbird², David N. Thompson³, and Mohammad S. Roni³

1 National Renewable Energy Laboratory

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3 Idaho National Laboratory

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Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-71949
November 2018



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Suggested Citation

Ryan Davis, Nicholas Grundl, Ling Tao, Mary J. Bidy, Eric C.D. Tan, Gregg T. Beckham, David Humbird, David N. Thompson, and Mohammad S. Roni. 2018. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Coproducts: 2018 Biochemical Design Case Update: Biochemical Deconstruction and Conversion of Biomass to Fuels and Products via Integrated Biorefinery Pathways*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-71949. <https://www.nrel.gov/docs/fy19osti/71949.pdf>.

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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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Executive Summary

The U.S. Department of Energy (DOE) promotes the production of an array of liquid fuels and bio-derived chemicals from lignocellulosic biomass feedstocks by funding fundamental and applied research that advances the state of technology in biomass collection, conversion, and sustainability. As part of its involvement in this program, the National Renewable Energy Laboratory (NREL) investigates the conceptual production economics of these fuels.

Over the past decade, NREL conducted a campaign to quantify the economic implications associated with observed and future targeted performance for the biochemical conversion of corn stover to ethanol through techno-economic modeling. This effort served to set “state of technology” benchmarks and to guide research and development by setting cost targets and tracking progress toward final achievement of these targets in 2012. Beginning in 2013, NREL began transitioning from the singular focus on ethanol to a broad slate of products and conversion pathways, generally focusing on drop-in hydrocarbon fuels or fuel blendstocks, ultimately to establish similar benchmarking and targeting efforts. Several earlier technical reports were released over 2013–2015 documenting initial strategies for achieving interim cost projections based either on biological or catalytic upgrading of lignocellulosic sugars, but with less quantitative focus on longer-term projections for ultimately achieving final hydrocarbon fuel cost goals. This report serves as an update to the biological sugar conversion approach, reflecting modifications to underlying conversion operational strategies, as well as refinements to the techno-economic model details. In addition, the report includes a more quantitative focus on envisioned processing requirements for achieving final fuel cost goals moving further into the future, via inclusion of value-added coproducts.

The overarching process designs evaluated here convert biomass to diesel- and naphtha-range fuels using alkaline and mechanical refining pretreatment, enzymatic saccharification, biological (fermentative) conversion of hydrolysate sugars to intermediate fuel precursors, and catalytic upgrading of those intermediates to final fuel products. Additionally, value-added coproducts—represented by adipic acid as a proof-of-concept example—are produced by the deconstruction and upgrading of lignin and other biomass residual components through a similar sequential biological and catalytic processing train. Ancillary areas—feed handling, hydrolysate processing, wastewater treatment, residual waste combustion, and utilities—are also included in the design. Broadly, the fuel production processes considered in this report are based on two example anaerobic pathway classes for bioconversion of hydrolysate sugars to hydrocarbon fuel intermediates, namely short-chain carboxylic acids and 2,3-butanediol (BDO), followed by catalytic upgrading steps to remove oxygen and undergo condensation/oligomerization reactions to produce longer-chain hydrocarbon fuel blendstocks. Aerobic bioconversion pathways to fuel components (e.g., lipid/fatty acid pathways) are not included in this design case, given more challenging design and economic constraints for such pathways in ultimately being able to achieve the required cost targets (on the order of roughly \$2/gallon gasoline equivalent (GGE) cost premiums previously estimated for aerobic versus anaerobic options). Detailed material and energy balances and capital and operating costs for this baseline process are also documented.

This techno-economic analysis models a production cost for cellulosic hydrocarbon biofuels that can be considered as a baseline to assess the competitiveness and market potential for the technology. It can also be used to quantify the economic impact of individual conversion

performance targets and prioritize them in terms of their potential to reduce cost. The analysis presented here also includes consideration of key environmental sustainability implications of the modeled biorefineries by tracking sustainability metric indicators such as carbon yields, primary energy import demands (natural gas and power imports), and water consumption attributed to the conversion process models. Additionally, an accounting of energy balances is provided, to quantify the energy output allocations across the biorefinery.

Building on prior design report practices, NREL, supported by subcontractor DWH Process Consulting, performed a feasibility-level analysis for a plausible integrated biorefinery conversion process to meet the ultimate DOE fuel selling price goal of \$2.50/GGE or less by the year 2030. The modeled biorefinery processes 2,205 dry tons biomass per day at a target price of \$71.26/dry ton (delivered to the pretreatment reactor throat) and achieves a fuel selling price of \$2.49/GGE for the “acids” pathway or \$2.47/GGE for the “BDO” pathway to fuels (2016 U.S. dollars) as determined by modeled conversion targets and “*n*th-plant” project costs and financing. These fuel price estimates are attributed to a total fuel yield of 44.8 and 43.2 GGE/dry ton for the acids and BDO pathways, respectively, as well as a final adipic acid coproduct yield of 259 and 266 lb/dry ton for the respective cases, with an adipic acid market value of \$0.86/lb. Additionally, given substantial demands for caustic (sodium hydroxide) and acid usage throughout the integrated process at considerable costs, this work highlights the need for either recovering and reusing these chemicals through advanced separations technologies, or otherwise offsetting a portion of those costs through the sale of the resultant sodium sulfate byproduct. The latter is reflected in this report, generating a smaller co-product revenue stream for sale of this salt at \$0.07/lb, beyond the purposeful co-production of adipic acid. All modeled fuel prices are also based on underlying financial assumptions including 10% internal rate of return, 40% equity financing (60% debt financing at 8% interest), and 30-year plant lifetime.

Both pathways exhibit high sensitivity to yields across the fuel production trains, but even more strongly to both yields and productivities for lignin deconstruction and bioconversion to coproducts, given both the high processing costs but also high value and thus revenue garnered from the lignin coproduct train as a key factor in achieving the fuel cost targets stipulated here. For achieving more near-term interim fuel selling price goals of \$3/GGE by 2022, simplistically assuming all other conversion process parameters remain fixed (aside from feedstock cost at \$79.07/dry ton for an interim 2022 target), the overall adipic acid coproduct yields could be relaxed by roughly 12% to 229 and 235 lb/dry ton for acids and BDO, respectively. Finally, the report includes a brief discussion on additional opportunities for future consideration that may further improve biorefinery economics, primarily alternative configurations for conversion of both carbohydrates and lignin to either fuels or products as well as opportunities for waste gaseous carbon utilization to improve overall carbon retention efficiencies.

Biological Renewable Diesel Blendstock (RDB) via Butyric Acids: Process Engineering Analysis
 DMR Pretreatment, Continuous Enzymatic Hydrolysis, Anaerobic Bioconversion, Catalytic Upgrading, Lignin Conversion to Coproducts

All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$2.49 /GGE**

Contributions:	Feedstock	\$1.59 /GGE
	Fuel Conversion	\$3.87 /GGE
	Coproduct Conversion	-\$2.97 /GGE

Fuel Production	32.5 MMGGE per year
Fuel Yield	44.8 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	259 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.43 [0.49] kg Acid/kg Total Sugars (89% of theoretical)
Feedstock + Handling Cost	\$71.26 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$48,653,825
Area 300: Sugar Hydrolysis and Conditioning	\$62,697,299
Area 400: Enzyme Production	\$11,526,084
Area 500: Bioconversion and Upgrading	\$43,799,229
Area 600: Wastewater	\$38,810,731
Area 700: Lignin	\$127,474,183
Area 800: Boiler	\$48,720,730
Area 900: Utilities & Storage	\$17,195,641
Total Installed Equipment Cost	\$398,877,721
Added Direct + Indirect Costs (% of TCI)	\$359,522,279 47%
Total Capital Investment (TCI)	\$758,400,000
Installed Equipment Cost/Annual GGE	\$12.28
Total Capital Investment/Annual GGE	\$23.35
Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.129
Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	49.9%
From Biomass (Fuel C / Biomass C)	26.2%
Adipic Acid Carbon Efficiency from Biomass	14.4%
Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr) ^b	99,659
Current Yield (Actual/Theoretical)	77.4%

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	158.9
Sulfuric Acid	24.2
Caustic	105.1
Glucose (enzyme production)	26.0
Hydrogen	0.0
Electricity (import)	72.9
Other Raw Materials	36.0
Catalysts	5.1
Waste Disposal	4.3
Na2SO4 Coproduct (\$0.07/lb)	-52.4
Adipic Acid coproduct (\$0.86/lb)	-493.1
Fixed Costs	61.5
Capital Depreciation	73.9
Average Income Tax	22.7
Average Return on Investment	204.0
Total	249.0

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$51,600,000
Sulfuric Acid	\$7,900,000
Caustic	\$34,100,000
Glucose (enzyme production)	\$8,400,000
Hydrogen	\$0
Electricity (import)	\$23,700,000
Other Raw Materials	\$11,700,000
Catalysts	\$1,700,000
Waste Disposal	\$1,400,000
Na2SO4 Coproduct (\$0.07/lb)	-\$17,000,000
Adipic Acid coproduct (\$0.86/lb)	-\$160,100,000
Fixed Costs	\$20,000,000
Capital Depreciation	\$24,000,000
Average Income Tax	\$7,400,000
Average Return on Investment	\$66,200,000
Total	\$81,000,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	10.9
Plant Electricity Use (kWh/GGE)	15.8
Metabolic Yield (g/g substrate)	
Glucose to Butyric	0.465
Glucose to Biomass	0.041
Xylose to Butyric	0.416
Xylose to Biomass	0.123
Arabinose to Butyric	0.418
Arabinose to Biomass	0.016

^a Complete conversion of biomass carbohydrates fuel

^b Recovered fuel yield after concentration, sent to hydrotreating (Theoretical yields above do not consider process recovery losses during product upgrading and purification)

Figure ES-1. Economic summary for anaerobic bioconversion via acids pathway

Biological Renewable Diesel Blendstock (RDB) via 2,3-Butanediol: Process Engineering Analysis

DMR Pretreatment, Whole-slurry Enzymatic Hydrolysis & Anaerobic Bioconversion, Catalytic Upgrading, Lignin Conversion to

Coproducts

All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$2.47 /GGE**

Contributions: Feedstock	\$1.65 /GGE
Fuel Conversion	\$3.83 /GGE
Coproduct Conversion	-\$3.00 /GGE

Fuel Production	31.3 MMGGE per year (at 68 °F)
Fuel Yield	43.2 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	266 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield]	0.45 [0.5] kg BDO/kg Total Sugars (90% of theoretical)
Feedstock + Handling Cost	\$71.26 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	Manufacturing Costs (cents/GGE fuel product)
Area 200: Pretreatment	Feedstock + Handling
\$48,653,825	164.9
Area 300: Sugar Hydrolysis and Conditioning	Sulfuric Acid
\$15,441,726	25.9
Area 400: Enzyme Production	Caustic
\$11,526,084	112.5
Area 500: Bioconversion and Upgrading	Glucose (enzyme production)
\$61,083,902	27.0
Area 600: Wastewater	Hydrogen
\$35,611,508	33.1
Area 700: Lignin	Electricity (import)
\$128,436,573	71.4
Area 800: Boiler	Other Raw Materials
\$50,985,372	33.7
Area 900: Utilities & Storage	Catalysts
\$15,506,286	9.4
	Waste Disposal
	4.5
	Na2SO4 Coproduct (\$0.07/lb)
	-55.6
	Adipic Acid coproduct (\$0.86/lb)
	-527.1
	Fixed Costs
	59.7
	Capital Depreciation
	70.6
	Average Income Tax
	21.8
	Average Return on Investment
	195.2
	Total
	247.1
	Manufacturing Costs (\$/yr)
	Feedstock + Handling
	\$51,600,000
	Sulfuric Acid
	\$8,100,000
	Caustic
	\$35,200,000
	Glucose (enzyme production)
	\$8,400,000
	Hydrogen
	\$10,400,000
	Electricity (import)
	\$22,300,000
	Other Raw Materials
	\$10,500,000
	Catalysts
	\$2,900,000
	Waste Disposal
	\$1,400,000
	Na2SO4 Coproduct (\$0.07/lb)
	-\$17,400,000
	Adipic Acid coproduct (\$0.86/lb)
	-\$164,900,000
	Fixed Costs
	\$18,700,000
	Capital Depreciation
	\$22,100,000
	Average Income Tax
	\$6,800,000
	Average Return on Investment
	\$61,100,000
	Total
	\$77,200,000

^a Complete conversion of biomass carbohydrates fuel

^b Recovered fuel yield after concentration, sent to hydrotreating (Theoretical yields above do not consider process recovery losses during product upgrading and purification)

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	10.7
Plant Electricity Use (kWh/GGE)	13.7
Metabolic Yield (g/g substrate)	
Glucose to 2,3-BDO	0.485
Glucose to Biomass	0.017
Xylose to 2,3-BDO	0.487
Xylose to Biomass	0.017
Arabinose to 2,3-BDO	0.478
Arabinose to Biomass	0.018

Figure ES-2. Economic summary for anaerobic bioconversion via BDO pathway

Nomenclature

ACCE	Aspen Capital Cost Estimator	SBL	inside-battery-limits
ACM	Aspen Custom Modeler	lb	pound
APR	aqueous phase reforming	LHV	lower heating value
BCD	base-catalyzed deconstruction	LCA	life cycle analysis
BDO	butanediol	MEK	methyl ethyl ketone
BETO	Bioenergy Technologies Office	MFSP	minimum fuel selling price
BTU	British thermal unit	MM	million
CEH	continuous enzymatic hydrolysis	MVR	mechanical vapor recompression
CHP	combined heat and power	MYPP	Multi-Year Program Plan
CIP	clean-in-place	NADH	nicotinamide adenine dinucleotide hydride
COD	chemical oxygen demand	NG	natural gas
CSL	corn steep liquor	NREL	National Renewable Energy Laboratory
CSTR	continuous stirred tank reactor	ORNL	Oak Ridge National Laboratory
DAP	diammonium phosphate	OTR	oxygen transfer rate
DDA	deacetylation and dilute acid	OUR	oxygen uptake rate
DMR	deacetylation and mechanical refining	R&D	research and development
DOE	U.S. Department of Energy	RCF	reductive catalytic fractionation
EH	enzymatic hydrolysis	RO	reverse osmosis
FGD	flue gas desulfurization	SMR	steam methane reforming
FCI	fixed capital investment	SOT	state of technology
gal	gallon	SS	soluble solids
GGE	gallon gasoline equivalent	TCI	total capital investment
GHG	greenhouse gas	TDC	total direct cost
HDO	hydrodeoxygenation	TEA	techno-economic analysis
HP	high-pressure	TOPO	tri-octyl-phosphine oxide
ILM	integrated landscape management	TS	total solids
INL	Idaho National Laboratory	WHSV	weight hourly space velocity
IRR	internal rate of return	WWT	wastewater treatment
IS	insoluble solids		

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1 Introduction

1.1 Background and Motivation

The U.S. Department of Energy (DOE) Bioenergy Technologies Office (BETO) promotes the production of liquid fuels from lignocellulosic feedstocks by sponsoring programs in fundamental and applied research that aim to advance the state of biomass conversion technology. These programs include laboratory research to develop improved bioconversion organisms, chemical catalysts, hydrolysis enzymes, and integrated unit operations through synthetic biology, catalyst development and testing, chemical and mechanical pretreatment work, detailed engineering studies of potential processes, and construction of pilot-scale demonstration and production facilities. This research is conducted by national laboratories, universities, and private industry in conjunction with engineering and construction companies.

To support the DOE program, the National Renewable Energy Laboratory (NREL) investigates the process design and economics of modeled cellulosic biorefineries in order to develop a plant gate price for fuels and fuel blendstocks based on process and plant design assumptions consistent with applicable best practices in engineering, construction, and operation. This plant gate price is referred to as the minimum fuel selling price or MFSP. The MFSP can be used by DOE to assess the cost-viability and market penetration potential of a given cellulosic biofuel technology pathway in comparison with petroleum-derived fuels and established biofuel technologies such as starch- or sugar-based ethanol. Ultimately, through techno-economic analysis (TEA), the modeled MFSP may be viewed as a bridge between understanding the process requirements from “bottom-up” modeling that must be achieved in order to meet DOE cost goals set from the “top down.”

The TEA effort at NREL also helps to direct biomass conversion research by examining the sensitivity of the MFSP to process alternatives and research advances. Proposed research and its anticipated results can be translated into a new MFSP that can be compared to the benchmark case documented in this report. Such comparison helps to quantify the economic impact of core research targets at NREL, and elsewhere, and to track progress as research evolves through “state of technology” benchmarking of MFSP reductions. It also allows DOE to make more informed decisions about research proposals that claim to reduce MFSP, and to better quantify trade-offs between process metrics (e.g., yields, chemical inputs, and carbon efficiencies), economics (MFSP), and sustainability (e.g., emissions and energy and water usage) among process options for a given technology pathway or amongst multiple pathways.

For more than 20 years, NREL developed design case models and associated reports [1-3] that documented process and cost targets for ethanol production from cellulosic feedstocks via biochemical conversion (e.g., deconstruction to monomeric sugars followed by fermentation to ethanol) based on the best understanding of the technology and equipment costs at the time. As understanding evolved on process and economic metrics, models were refined and re-benchmarked relative to updated targets. The final update to the ethanol design targets was published in 2011 (referred to hereafter as the *2011 design report*) [2] and established an MFSP cost goal of \$2.15/gal ethanol (\$3.27/gal gasoline equivalent (GGE), 2007 U.S. dollars) to be achieved in 2012 based on performance data from pilot-scale demonstration runs conducted at NREL. This goal was subsequently achieved through 2012 pilot plant trials, with the pertinent experimental data input to the model, which calculated an ethanol MFSP of \$2.15/gal for a

commercial-scale “*n*th-plant” facility processing 2,000 dry metric tons/day of corn stover [4-6]. Further context on the history of NREL’s ethanol program, including individual year-by-year modeled production costs, may be found in published NREL reports [5, 7].

Following the 2012 ethanol demonstrations, all BETO platforms began to transition in focus toward hydrocarbon fuel and blendstock products (fungible/infrastructure-compatible fuels), including a new pathway MFSP target of \$3/GGE by 2022 [8]. Within the biochemical platform, two pathway design cases were initially established to document possible strategies to achieve future hydrocarbon MFSP goals, based on a biological sugar conversion pathway (via aerobic fatty acid production and upgrading) and a catalytic sugar conversion pathway (via aqueous phase reforming and upgrading of hydrolysate sugars) [9, 10]. Both cases focused primarily on production of fuels from biomass carbohydrates, which in isolation only stood to achieve MFSPs on the order of roughly \$5/GGE, and as such were viewed as interim projections for a shorter timeframe prior to 2022. Both cases also highlighted that to ultimately achieve \$3/GGE or lower MFSP targets, it would be necessary to utilize more of the biomass, namely lignin and other under-utilized components, for production of value-added coproducts.

At the time, specific details were not yet well-understood on what such lignin coproduct trains would look like, but a higher-level sensitivity analysis was provided on feasibility TEA estimates for four example coproduct options. The two example components that maintained oxygen in their structures (adipic acid and 1,4-butanediol) were shown to be superior choices both from an economic and environmental sustainability standpoint. This highlighted a key advantage for bio-derived products, namely that maintaining oxygen (a) increases overall mass of the coproduct as well as atom efficiency from the starting biomass and (b) allows for less energy-intensive methods to produce such coproducts. This second advantage is due to the presence of oxygen in the starting biomass, as petrochemical routes must undergo costly and energy-demanding synthesis steps to add oxygen from initial oxygen-free petroleum feedstocks [11]. Alongside such coproduct considerations, market size is also a key factor as the coproduct must exceed small niche market volumes in order to avoid saturating existing product markets to support commodity scale deployment of such biorefineries; this is further discussed later in Section 5.2.3 for the coproduct evaluated in this work.

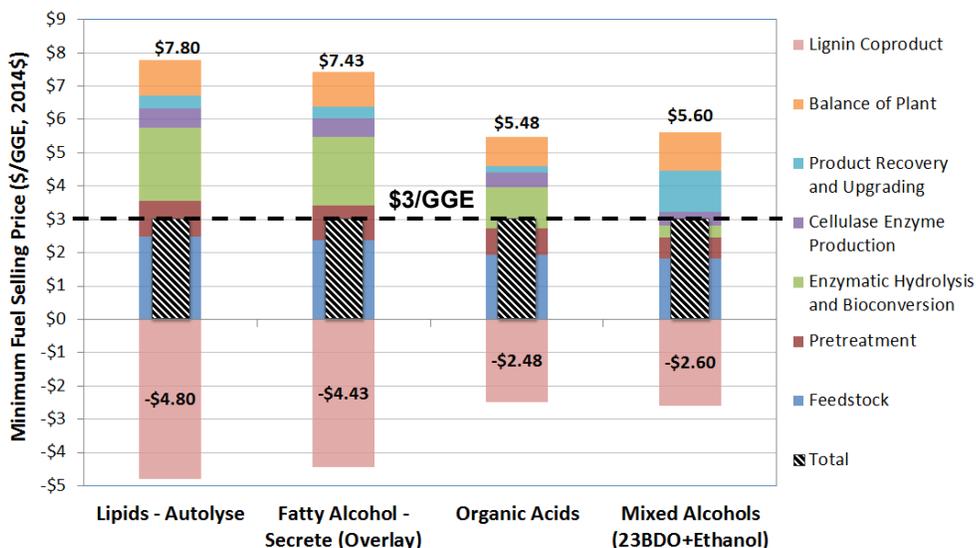
Historically, the primary focus in NREL’s biochemical platform has been on biological conversion routes, although catalytic and hybrid approaches have also become more emphasized in recent years under the Chemical Catalysis for Bioenergy Consortium (<https://www.chemcatbio.org>) and other efforts. Thus, following the initial design cases noted above, the majority of experimental and TEA activities were focused on bioconversion to fuel precursors. NREL’s 2013 “biological design report” targeted the production of fatty acids, produced via aerobic bioconversion of sugars, with the assertion that the fatty acids would be made to be secreted from the cell in order to avoid costly intracellular extraction steps [10]. However, once experimental efforts began to take shape after publication of the report, it became apparent that meeting the stipulated targets for fatty acid yields, fermentation productivities, and product secretion would pose major challenges to be achieved in a short timeframe. Accordingly, in 2014 a new process was developed termed the “C5/C6” pathway, whereby hemicellulose sugars (produced following dilute acid pretreatment) were separated from the cellulose and other solids components and fermented to succinic acid as a coproduct in parallel to fuel production from the glucose (cellulose) fraction. This configuration allowed for relaxing the targets for the

fuel train bioconversion step, instead based on production of oleaginous yeast with intracellular accumulation (and subsequent extraction) of lipids, while still maintaining similar MFSP goals as the prior fuel-only approach enabled by the coproduct revenue from succinic acid [11].

Following establishment of the C5/C6 pathway TEA models, NREL's experimental efforts moved to focus on this concept over the period of 2014–2015. Over this short timeframe, significant progress was demonstrated for both the C6 (fuel) and C5 (succinic acid) processes, which translated to a roughly \$5/GGE reduction in modeled benchmark state of technology (SOT) MFSPs in that time [12]. However, as this pathway was generally viewed as a short-term strategy to an intermediate cost goal (after which point the process would again be changed to move to final cost targets in the longer-term), at BETO's direction in 2015, the C5/C6 pathway was de-emphasized to begin focusing on such longer-term goals for ultimately demonstrating cost targets into 2022 and beyond. Thus, NREL's TEA efforts were again exercised to understand the requirements in more detail for the technical targets that would be necessary in order to achieve \$3/GGE MFSPs or lower over such timeframes.

Through 2016–2017, the modeling and experimental work initially focused on four representative bioconversion pathway options for conversion of sugars to fuel precursors, namely oleaginous yeast lipids (aerobic), fatty alcohols (aerobic), carboxylic acids (anaerobic), and 2,3-butanediol (BDO) (anaerobic/minimal oxygen required for cell redox balancing). TEA screening indicated that all four pathways exhibited the technical potential to achieve \$3/GGE MFSPs, albeit all would require substantial assistance from lignin coproducts (consistent with prior findings noted above), but significantly more so for the aerobic cases relative to anaerobic (Figure 1, where the bottom negative bar represents the coproduct revenues required from lignin inclusive of lignin coproduct processing costs). This was due to inherently lower energy (GGE) yields and higher processing costs for aerobic bioconversion compared to anaerobic, with the latter tied to the costs of delivering and solubilizing oxygen to an aerobic bioreactor [13].

Additional anaerobic options are also possible, most simplistically also including a maintained focus on ethanol as an intermediate for catalytic upgrading to hydrocarbons (in fact ethanol was originally co-produced alongside 2,3-BDO in early *Zymomonas* engineering efforts, incurring a separate catalytic upgrading train in parallel with BDO [14]). An ethanol-to-hydrocarbon pathway may be envisioned to offer further cost advantages than even acids or BDO, being a more simplistic and established technology (and with higher potential energy yields across fermentation), but for this same reason also may offer less opportunities for new research advancements to be made. Additionally, intermediate molecules such as carboxylic acids and BDO also offer more versatility in pursuing opportunities for conversion to both fuels and value-added products, which may allow for more flexibility in operating a biorefinery to focus on fuels or products as conditions dictate.



Metric	Lipids	Fatty Alcohols	Organic Acids	BDO + EtOH
MFSP (\$/GGE, 2014\$) – prior to coproducts	\$7.80	\$7.43	\$5.48	\$5.60
Fuel C efficiency from biomass (%)	20%	21%	25%	27%
Fuel yield (GGE/ton)	34.2	35.7	43.5	46.5
TCI (\$MM) – prior to coproducts	\$640	\$628	\$520	\$527
Fuel carbon chain length	~14-20	~16-20	~11-14	~8-18
Carbon efficiency through lignin-to-coproduct train required to achieve \$3/GGE (C in adipic acid vs C available in residual biomass)	59%	56%	40%	46%

Figure 1. Summary of MFSP and TEA metrics for four representative fuel bioconversion pathways

After reverting back from the C5/C6 pathway to whole-sugar conversion to fuels, from 2015 to 2016, NREL experimental efforts continued focusing primarily on the yeast lipids pathway, at least within the context of integrated biochemical processing. This pathway was chosen because it was the most established case with a history of experimental work on variants of this approach since 2013, relative to other pathways indicated in Figure 1. All other pathways were in earlier stages of research and generally based on clean sugars. Over that time, substantial experimental progress continued to be made, notably the achievement of a roughly \$1.50/GGE reduction in modeled MFSP in the 2016 SOT for whole sugar conversion relative to 2015 for the C5/C6 pathway. This was achieved by compensating for the loss of the valuable succinic acid coproduct with a significant improvement in enzymatic hydrolysis and lipid fermentation performance including a doubling in lipid fermentation productivity while increasing lipid yield by 26%, which was even further improved in 2017 [12].

Despite these historical achievements, the decision was made in 2018 (preceding this design report) to transition away from the lipids pathway (and aerobic pathways as a whole) in favor of moving to the anaerobic pathway cases shown in Figure 1. This decision was based on the more challenging route to achieve \$3/GGE by 2022, which more recently has been further extended to below \$2.50/GGE by 2030, in light of the recent decline in oil prices which dictate “cost viability” for biofuels. Such cost targets place significantly more burdens on the requirements from lignin coproducts (or alternative cost reduction needs) to overcome a cost premium of \$2/GGE or more between aerobic versus anaerobic pathways prior to reflecting lignin

coproducts. Further discussion on the “aerobic versus anaerobic” tradeoffs from a TEA modeling standpoint is included in Section 3.5. In this context, the overall scope of this report focuses on model details attributed to achieving final MFSP costs of \$2.50/GGE or less by 2030 for both anaerobic fuel train pathways (acids and BDO intermediates), evaluated as two separate process configuration approaches, with additional qualitative discussion at the end of the report on additional process configuration options that may also achieve similar or lower cost targets as may be considered in the future.

1.2 Process Overview

As noted above, **two separate process cases** are considered in this report based on fermentation pathway to the fuel precursor intermediate, namely carboxylic acids and BDO. The pathways share numerous steps in common outside of the fuel fermentation/upgrading operations, but there are also several distinctions to optimize overall process integration, discussed throughout the report. The processes modeled here use deacetylation/mild alkaline extraction and mechanical refining pretreatment of lignocellulosic biomass feedstock (primarily corn stover), followed by enzymatic hydrolysis (saccharification) of the cellulose and xylan, followed by hydrolysate concentration and bioconversion in the acids case or directly to bioconversion in the BDO case. The bioconversion intermediates (acids/BDO) are subsequently catalytically upgraded to final hydrocarbon fuel products. Lignin is deconstructed to soluble monomers and converted (along with other biomass residual components) to muconic acid which is purified and further upgraded to adipic acid for sale as a coproduct. The facility also includes feedstock handling and storage, wastewater treatment (WWT), residual waste combustion, product storage, and utilities. The process is divided into nine areas (Figure 2).

Area 100: Feedstock logistics and handling. The feedstock, in this case blended herbaceous biomass (primarily corn stover), is delivered to the feed handling area from a uniform-format feedstock supply system. All Area 100 processing aspects are outside the scope of this work, and are rolled into delivered feedstock costs at the throat of the pretreatment reactor (Area 200).

Area 200: Pretreatment. In this area, the biomass is processed in a continuous alkaline extraction/deacetylation step to solubilize and remove acetate as well as portions of ash, lignin, and other components (also incurring some losses of carbohydrates). The process utilizes counter-current extraction with recycling of the caustic liquor. The exiting solids are squeezed in a screw press to increase solids content to 30 wt% and then sent to mechanical refining to open biomass fibers for increased enzyme accessibility through enzymatic hydrolysis.

Area 300: Enzymatic hydrolysis and hydrolysate conditioning. In the BDO case, enzymatic hydrolysis is initiated in a high-solids continuous reactor using a cellulase enzyme produced on site. The partially hydrolyzed slurry is sent to one of several parallel batch reactors. Hydrolysis is completed in the batch reactor with a total time of 5 days between the continuous and batch steps. The whole-slurry hydrolysate is then cooled and directly fermented in the same batch reactors (associated fermentation tankage volume is allocated under A500). In the acids case, the pretreated material is sent through a continuous enzymatic hydrolysis (CEH) process based on a series of hydrolysis reactors each connected through a pump-around loop to filtration units to continuously remove sugars prior to sending residual solids to the next hydrolysis tank. The final remaining hydrolysate stream from the last reactor is sent through a lignin press with the liquor

combined with the filtrate from the other steps, while the solids fraction is routed to the lignin train. The clarified liquor is concentrated in a mechanical vapor recompression evaporator and then routed to acids fermentation.

Area 400: Enzyme production. An on-site enzyme production section was maintained in this design, consistent with details provided in prior design reports. Purchased glucose (corn syrup) is the primary carbon source for enzyme production, in this case producing enzymes for both cellulose and hemicellulose saccharification. An enzyme-producing fungus (modeled after *Trichoderma reesei*) is grown aerobically in fed-batch bioreactors. The whole fermentation broth, containing the secreted enzyme, is fed to Area 300 to carry out enzymatic hydrolysis.

Area 500: Fermentation, catalytic conversion, and upgrading. In the BDO case, the hydrolysate is cooled and directly subjugated to whole-slurry fermentation. The fermentation broth is then sent to a lignin press to remove lignin and other insoluble solids, and the clarified stream is routed to aqueous BDO upgrading, yielding butene and minor byproducts. The butene is distilled from the water and then further upgraded through oligomerization and hydrotreating steps to finished hydrocarbon fuels primarily in the diesel range. In the acids case, fermentation is done on clarified hydrolysate in a similar fermentor vessel as used for BDO, but with a pumparound loop through a membrane to isolate acids into a solvent system located on the other side of the membrane (pertractive recovery). The solvent is subsequently recovered and recycled via distillation, and the acids are then upgraded through a series of ketonization, condensation, and hydrotreating steps to hydrocarbon fuels in the diesel range.

Area 600: Wastewater treatment. Wastewater streams (primarily aqueous broth after recovery of fermentation intermediates in Areas 500 and 700) are treated by aerobic digestion and reverse osmosis to remove organics and salts, respectively. Anaerobic digestion is not utilized in this design given substantially lower chemical oxygen demand (COD) loading levels entering Area 600 than in prior cases. The treated water is suitable for recycling and is returned to the process. Sodium sulfate salt recovered from the brine is sold as a secondary coproduct to offset a portion of the caustic and acid demands/costs incurred throughout the integrated design.

Area 700: Lignin upgrading. The black liquor from deacetylation and mechanical refining (DMR) pretreatment is combined with the residual solids separated either during CEH (acids case) or following fermentation (BDO case) and routed to a more severe base-catalyzed deconstruction (BCD) step to solubilize lignin to monomeric components. The lignin monomers, along with other residual (soluble) biomass components, are upgraded through bioconversion to muconic acid, which is then purified and hydrogenated to adipic acid. The adipic acid is recovered through crystallization to a finished coproduct.

Area 800: Combustor, boiler, and turbogenerator. The residual solids, wastewater sludge, and off-gas streams are combusted to generate high-pressure steam for heat and power. Excess steam beyond facility heating demands is converted to electricity for use in the plant.

Area 900: Utilities. This area includes a cooling water system, chilled-water system, process water manifold, and power systems.

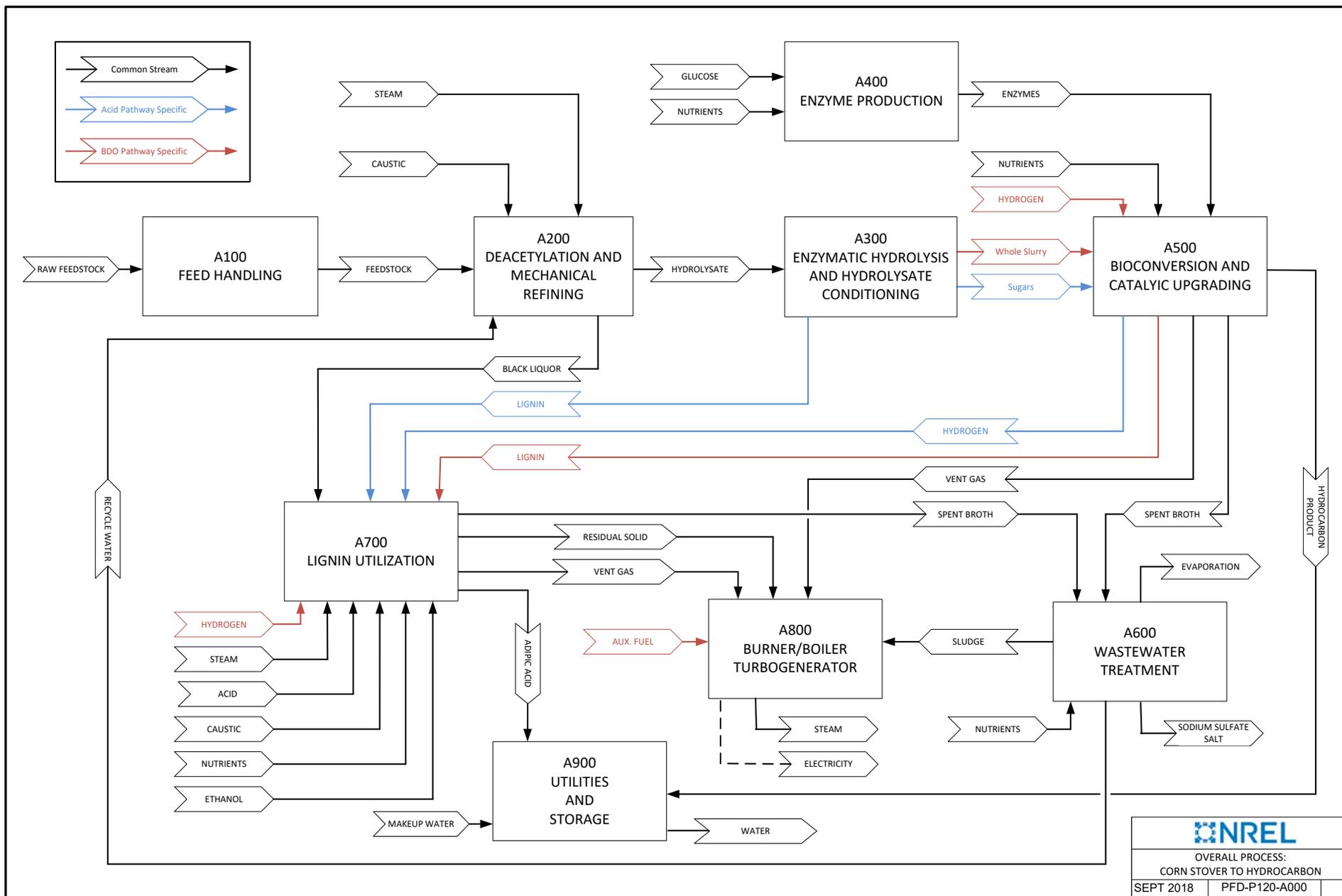


Figure 2. Simplified flow diagram of the overall process. (Key streams only. See Appendix D for more detailed schematic and process flow diagrams.)

1.3 Techno-Economic Analysis Approach and Assumptions

The engineering approach taken in this work for modeling the conversion process is similar to that described in prior design cases, and will not be repeated in the same detail here [9, 10]. In summary, process flow diagrams are initially developed based on inputs and discussions with researchers around pertinent process configurations (i.e., block flow diagram in Figure 2 and more detailed diagrams provided in Appendix D) from which process simulations are developed in Aspen Plus [15]. This software computes thermodynamically rigorous material and energy balances for each unit operation in this conceptual biorefinery. The material and energy balance data from the Aspen simulation are used to assist in determining the number and size of capital equipment items. As process conditions and flows change, baseline equipment costs are automatically adjusted in an Excel spreadsheet using a scaling factor. These baseline costs come from vendor quotes (a favored procedure when available for larger or nonstandard unit operations and packaged or skid-mounted subsystems), NREL and subcontractor historical cost data, or published engineering literature (when necessary). Final equipment costs for this report are tabulated in Appendix A.

Once equipment costs are determined, direct and indirect overhead cost factors (e.g., installation costs and project contingency) are applied to determine a feasibility-level estimate of total capital investment (TCI) in 2016\$. The TCI, along with the plant operating expenses (also developed using flow rates from the Aspen model), is used in a discounted cash flow rate of return (DCFROR) analysis to determine a plant gate price for total fuel at a given discount rate. The plant gate price, also called the minimum fuel selling price (MFSP), is defined as the sales price (in \$/GGE) required to obtain a net present value (NPV) of zero for a 10% internal rate of return (IRR) after taxes for a hypothetical n^{th} -plant model over a 30-year plant lifetime.

The product of the analysis is a techno-economic model that estimates a rational price for a pre-commercial process. The resultant MFSP is unique for the set of process conditions simulated, and it should be emphasized that some amount of uncertainty always exists around these chosen conditions, as well as around the assumptions made for capital and raw material costs. The underlying cost estimates and TEA modeling approach generally fall within an “engineering feasibility” level of analysis (generally AACE Class 4 [16]), with an expected uncertainty of approximately $\pm 25\%$ in the TCI estimates [17] (sensitivity to this and other parameters are considered in Section 5.2). Without a detailed understanding of the basis behind it, the computed MFSP carries a risk of being taken out of context. While the MFSP can be used to assess the marketplace competitiveness of a given process, it is best suited for comparing technological variations against one another or for performing sensitivity analyses that indicate where economic or process performance improvements are needed.

The analysis reported here assumes n^{th} -plant economics. The key assumption implied by n^{th} -plant economics is that our analysis does not describe a pioneer plant; instead, it assumes several plants using the same technology have already been built and are operating. In other words, it reflects a mature future in which a successful industry of n plants has been established. Because the techno-economic model is primarily a tool for studying new process technologies or integration schemes to comment on their comparative economic impact, n^{th} -plant analysis avoids artificial inflation of project costs associated with risk financing, longer startups, equipment overdesign, and other costs associated with first-of-a-kind or pioneer plants, lest these overshadow the economic impact of the technical research advances in conversion or process integration. While these n^{th} -plant economics may not be

reflective of pioneer plants and other early technology adopters, they should still help to provide justification and support the underlying technology.

The n^{th} -plant assumptions in the present model apply primarily to the factored cost model used to determine the total capital investment from the purchased equipment cost and to the choices made in plant financing. The n^{th} -plant assumption also applies to some operating parameters, such as an assertion of 90% process uptime (roughly 329 days operating per year); while some industries such as corn wet milling may operate as high as 96% uptime, 90% is viewed here as a reasonable n^{th} -plant target for a relatively complex integrated biorefinery as reflected in this effort. No concessions are included for equipment over-design, beyond standard redundancy included for some equipment such as compressors. These assumptions were agreed upon by BETO and reflect standard metrics applied universally across multiple national laboratory TEA models to allow for a consistent basis for analysis. It should be emphasized, however, that these assumptions carry a degree of uncertainty and are subject to refinement.

While Aspen Plus is thermodynamically rigorous, such detail is not always warranted in the simulation, whether for lack of data or introduction of additional complexity for little gain in accuracy. Some operations, such as membranes and other solid-liquid separations, were modeled as user defined unit operation modules with a fixed performance based on empirical data or by standard engineering practices. Catalytic reactors were modeled using stoichiometric reactions of discrete feed and product components rather than rigorous kinetics or rate expressions, which satisfies mass balances and appropriate reactor sizing when coupled with targeted catalyst space velocities. The Aspen Plus simulation uses component physical properties internal to the software, as well as property data developed at NREL or from the literature [18, 19]. Similar to prior recent models, the current model does not rely on external property databanks and minimizes the number of custom-defined components within reason (however, the same type of information is still maintained within the model file itself, i.e. no critical information is lost by eliminating use of external databanks). More details on historical components and their modeled properties may be found in prior design reports [2], [9, 10].

2 Design Basis and Conventions

2.1 Plant Size and Feedstock Specifications

The plant size in the present design is the same as that used in prior designs: 2,205 dry U.S. tons/day (2,000 metric tonne/day). With an expected 7,880 operating hours per year (90% uptime), the annual feedstock requirement is 724,000 dry U.S. tons/year. Given the focus on reducing both feedstock and conversion costs in support of the \$2.50/GGE MFSP goals, NREL and Idaho National Laboratory (INL) conducted initial analyses around feedstock/biorefinery scale, and found that moving to smaller scales (which reduces feedstock transportation costs) continues to be outweighed by biorefinery economy-of-scale penalties, consistent with prior indications from ethanol process modeling work [3]. Thus, at present, the 2,000-dry-metric-tonne/day basis continues to be maintained reflecting n^{th} -plant commercial scale.

Also consistent with prior recent design cases [3, 9, 10], the delivered feedstock composition is left unchanged. This composition was established reflecting previous INL target specifications developed around a uniform-format feedstock supply system, based on blended biomass composed of corn stover and switchgrass [20]. Moving forward, INL's strategies and future targets are evolving with respect to biomass blends and preprocessing logistics in order to further minimize delivered feedstock cost. While it is premature to establish the resulting compositional details of such new strategies (which will be forthcoming in future INL feedstock design cases), at a minimum, the target specifications will be maintained to meet or exceed 59% carbohydrates and 15.8% lignin. The feedstock composition assumed in the conversion model is shown in Table 1. In contrast to prior design cases that still focused only on carbohydrates (cellulose and hemicellulose), other components are of similar importance in the present model configurations, notably including lignin and acetate, given the modifications made for inclusion of the ability to upgrade these components to high-value coproducts.

Also of increasing merit in the present design is the component labeled “extractives.” The extractives fraction represents the nonstructural component fractions from the compositional analysis, some of which account for analytical mass balance closures below 100%, but otherwise are composed of simple organic components primarily in the form of sugars (e.g., glucose and fructose), sugar alcohols (e.g., glycerol and xylitol), and organic acids (C4–C6 acids) [21]. The amount and type of extractives in the biomass depends on the location and time of harvest, storage/processing logistics, and, in part, how much microbial degradation of the material occurs after harvest; the amount of extractives in a given sample may therefore be indicative of its age. Although the extractives component is thus more variable than other biomass constituents, its largely simple organic disposition makes it more important for the present and future biorefinery designs that are increasingly targeting utilization of the “whole” biomass for economical conversion to products. Thus, this component is also considered for its utility to be used in the lignin-to-coproducts train, rather than being considered a waste and handled in wastewater treatment as in prior design cases (discussed later). Sucrose is another extractive component, but it is measured separately in laboratory analysis and has been added as a separate feedstock component in the present design. The amount of sucrose present in the biomass is dependent on harvesting and handling practices. Although not pursued for economic value, the ash component may also merit further investigation regarding speciation of ash constituents to better understand potential implications on materials of construction (e.g. related to chloride) or to downstream catalyst activity (e.g. ash constituents that may pose high risk for catalyst poisoning).

Table 1. Delivered Feedstock Composition Assumed in the Present Design

Component	Composition (dry wt %)
Glucan	35.1
Xylan	19.5
Lignin	15.8
Ash	4.9
Acetate ^a	1.8
Protein	3.1
Extractives	14.7
Arabinan	2.4
Galactan	1.4
Mannan	0.6
Sucrose	0.8
<i>Total structural carbohydrate</i>	<i>59.0</i>
<i>Total structural carbohydrate + sucrose</i>	<i>59.8</i>
<i>Moisture (bulk wt %)</i>	<i>20.0</i>

^a Represents acetyl groups present in the hemicellulose polymer, converted to acetic acid under low-pH conditions.

In this design report update, the 2030 target delivered feedstock cost is set to \$71.26/dry U.S. ton (2016\$) based on guidance from partners at INL, reflective of all pre-processing costs through delivery to the “throat of the reactor” in the biorefinery. This represents a roughly 16% cost reduction relative to prior 2017 targets at \$85.06/ton (2016\$, originally \$84/ton in 2014\$), which were subsequently met based on INL’s 2017 state of technology demonstrations. More specific details attributed to feedstock logistics and future R&D plans in support of this cost target will be documented through INL feedstock design report updates in the future (this report precedes that from INL), but a brief discussion around general strategies for achieving this target is provided in Section 3.1.

2.2 Updated Modeling Basis

In keeping with prior recent design report updates, a number of underlying model parameters are maintained consistently in the present work. These include a 0.5-year facility startup time and 90% process uptime (7,884 hours per year on-stream factor). It should be emphasized that these are reflective of the n^{th} -plant modeling basis employed here, as discussed above, and early pioneer plants may require significantly longer startup times or sustain shorter annual uptimes. Other conventions such as reported units and physical quantities, like total solids (TS) and insoluble solids (IS), are consistent with details described previously [9, 10].

The results from this analysis are reported primarily in terms of energy yields in gallons gasoline equivalent, e.g., \$/GGE, GGE/yr, and GGE/ton. This includes energy yield in both the diesel and naphtha product cuts from hydrotreating distillation, rather than yield of a single product with the other treated as a coproduct. This is done to maintain focus on total fuel (energy) yield from biomass carbon, to avoid introducing unnecessary subjectivity in decisions for distillation column product cuts, or over-interpreting the current projections for catalytic upgrading steps with regards to catalyst selectivity to diesel over naphtha. Additionally, as the product distributions are different between the two sugar fuel train pathway approaches (acids and BDO), and even can be different among multiple options for intermediate upgrading within a single given pathway, to maintain consistent grounds, all yields and MFSPs are normalized to the GGE basis according to their energy content. Lower heating values (LHVs) for both diesel- and naphtha-range products were calculated by the Aspen model, and correspond to similar values for standard petroleum-equivalent products [22]. To translate to a GGE basis, a conventional gasoline heating value of 116,090 BTU/gal (LHV basis) was applied [22].

3 Process Design and Cost Estimation Details

3.1 Area 100: Feedstock Logistics and Handling

Feedstock logistics include operations that take place after the biomass is produced in a field or forest, but before it is introduced into a conversion process. All activities related to feedstock logistics are directed at reducing the delivered *cost* of sustainably produced feedstock, improving and preserving the *quality* of harvested feedstock to meet the needs of biorefineries, and/or expanding the *volume* of feedstock materials accessible to the bioenergy industry. Feedstock logistics efforts are primarily focused on identifying, developing, demonstrating, and validating efficient and economic systems to harvest, collect, transport, store, and preprocess raw biomass from a variety of crops to reliably deliver high-quality, high-volume, affordable feedstocks to biorefineries. Previous details associated with feedstock logistics, as well as feedstock compositional goals, have been documented in prior design reports [10], and future projection details will be published in a forthcoming design report by INL. This report precedes INL's and we defer to their future report to document the details of future feedstock logistics targets (which are otherwise outside the scope of the present TEA focus on biorefinery conversion); however, here we outline options based on inputs from INL which could further reduce the overall price associated with biomass while still maintaining the desired quality and property requirements to deliver a feedstock ready for the throat of reactor.

Feedstock has a large impact on the overall MFSP of biofuels, thus, reductions in feedstock costs can have a significant role in driving down the costs of biofuels and meeting future MFSP goals below \$2.50/GGE. A reduction in feedstock price to \$71.26/dry short ton (2016\$) would support this cost goal. Reducing the feedstock access cost is a key opportunity for further cost reductions. The farm gate cost is composed of the costs of establishing the crop (for perennial energy crops); harvest, collection, and road-siding the biomass; and a "grower payment" that represents the nutrient replacement cost and a grower profit incentive [23]. Opportunities for reducing these costs focus around utilizing more/different types of biomass to allow greater aggregate biomass to be available lower on the supply curve. Utilization of dedicated energy crops with increased yields that can also be managed independently of row-crop commodities allows new, more cost-effective logistics compared prior herbaceous feedstock logistics approaches.

Additionally, cost will be reduced through the utilization of low-cost, low-quality but readily available waste materials such as municipal solid waste (e.g., yard wastes). To utilize these materials, additional preprocessing and/or blending will be incorporated to meet conversion specifications. Improving quality will enable reduced dockage for not meeting conversion specifications and thus lower feedstock costs. Integrated landscape management (ILM) will be considered as both a method of increasing biomass supplies while affording the opportunity to offset grower costs with additional revenue sources. ILM is a promising strategy to reduce grower payments by increasing grower profitability through sustainable production practices, while increasing the availability of biomass by integrating high-yielding energy crops into unprofitable subfields [24]. ILM is increasingly recognized for its potential for sustainable food and energy production and additional benefits of improved ecological functions [25-29].

Another opportunity for lowering feedstock costs is to reduce losses of convertible material during harvest, collection, and storage. Losses in storage are quite high for herbaceous feedstocks in particular, averaging as much as 12%. Storage losses are the primary factor leading to a requirement to purchase 15% more biomass than reaches the reactor throat. Reducing these losses through approaches

such as field-side or local depot-located grinding and high-moisture densification is a potential cost trade-off that will be explored. In addition, inventory management strategies will be developed to target the highest moisture biomass for conversion soon after harvest.

Relatively inexpensive preprocessing technologies, such as air classification and size classification, have been shown to be effective for separating lower-quality fractions from the bulk of the biomass [30], as well as for separating individual plant tissues [31, 32], and will contribute to the cost reduction by separating out potential higher-value coproduct streams to offset production of biofuel. Fractional milling during continuous grinding processes can be used to separate specific fractions based on the quality and specific use for each fraction [33]. Chemical preprocessing has also been shown to be effective for removing conversion inhibitors [34], which could then be recovered as coproducts. In this way, the carbon efficiency of the overall field-to-biofuel system could be profitably improved. Intermediately preprocessed biomass fractions could be diverted from the primary conversion system to another system for which the fraction is better suited (for example, solubilizing lignin for routing to the biorefinery lignin train, leaving carbohydrate-enriched biomass to be routed directly to biorefinery pretreatment/hydrolysis). This may allow increased carbon utilization potential within respective fuel and coproduct trains.

Supply system intensification is another area that will be analyzed for the potential for feedstock cost reductions. New strategies that move preprocessing operations to the field, such as size reduction, can reduce both capital and energy costs for feedstock preprocessing at the biorefinery, including the field-side grinding/densification and forage chopper strategies described above. Opportunities for process intensification in preprocessing operations exist through the integration of drying with size reduction and densification. BETO-funded R&D has shown that drying requirements are greatly reduced through the use of wet fractional milling and high-moisture densification [35-39]. Further potential cost reductions include utilization of different types of mills and improving drying efficiency of loose biomass and high-moisture pellets using low-temperature drying technologies. Finally, utilization of existing commodity feed handling infrastructure will offer significant cost savings through the use of pelleted or briquetted feedstocks.

3.2 Area 200: Pretreatment

3.2.1 Overview

Pretreatment is accomplished in the current design by way of deacetylation and mechanical refining (DMR). Here, what is termed “deacetylation” is a somewhat more severe alkaline extraction operation, targeted to also remove more lignin in addition to acetyl groups. This enables more effective enzymatic hydrolysis compared to what had originally been reflected for this step when intended to primarily remove acetate under earlier configurations employing deacetylation and dilute acid (DDA) pretreatment in prior NREL TEA models [9, 10, 40]. The move from DDA to DMR pretreatment in this update is driven by two factors. First, the ability to use a low-pressure pretreatment operation avoids logistical and operational challenges that may be incurred at commercial scale for feeding biomass across a high-pressure envelope, while avoiding the use of acid, resulting in cleaner sugars with less inhibitors for improved hydrolysis and fermentation yields [41]. Second, the inclusion of lignin upgrading to coproducts necessitates DMR as DDA pretreatment renders the lignin generally unconvertible through downstream deconstruction/conversion operations [42, 43].

Following alkaline extraction, DMR employs the use of a two-stage mechanical processing operation, namely disc refining followed by a secondary roller mill as shown in see Figure 3. Rather than chemically hydrolyzing fractions of the biomass (primarily hemicellulose) in the case of DDA pretreatment, these mechanical steps delaminate and defibrillate the biomass structure, thereby increasing the surface area of the biomass for improved cellulose and hemicellulose access to enzymes [41]. Additionally, the DMR process enables higher sugar concentrations than DDA after downstream enzymatic hydrolysis at equivalent TS loading levels, given lower levels of other components such as salts and degradation products (this can be seen in NREL’s recently-updated sugar model, available publicly from <https://www.nrel.gov/extranet/biorefinery/aspen-models/>).

In the present envisioned design, a continuous counter-current extraction unit is employed that feeds biomass and a caustic solution at opposite ends of a screw conveyor, with the resulting liquor phase routed to the lignin upgrading train and the solids phase sent on to mechanical refining and then downstream enzymatic hydrolysis.

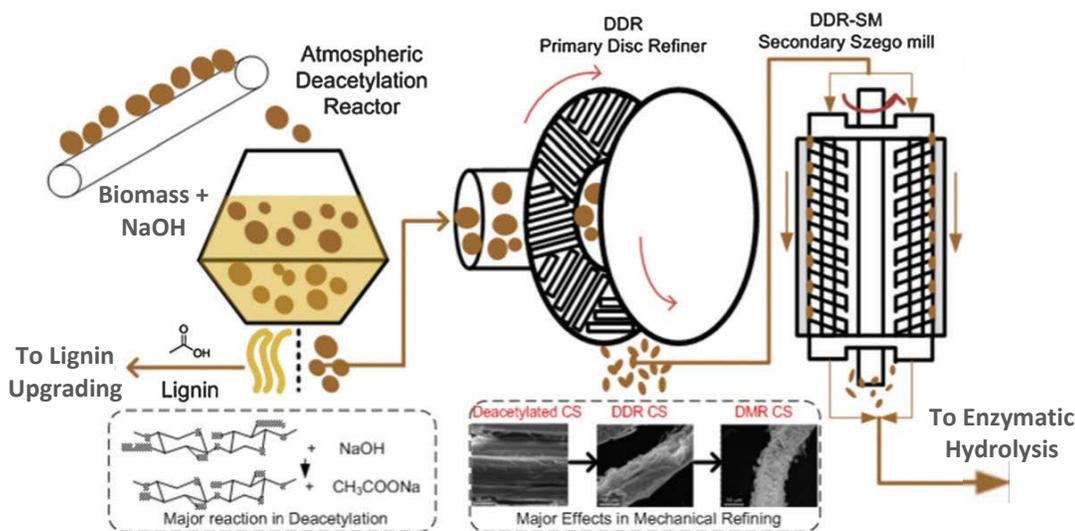


Figure 3. Schematic diagram of key DMR process operations (adopted from [41]). In this example diagram, the deacetylation/dilute alkali step is represented as a batch reactor, but is modeled in the present work as a counter-current alkaline extraction unit with internal recycle of the black liquor.

3.2.2 Design Basis

The deacetylation/alkaline extraction step is modified in several ways relative to the design described in prior cases [10]. First, the severity of the operation is increased in terms of caustic loading (70 mg/g dry biomass feed versus 17 mg/g used previously for DDA pretreatment), temperature (92°C versus 80°C), and residence time (90 versus 60 minutes) as required to support sufficient acetate/lignin removal for downstream efficacy of mechanical refining and enzymatic hydrolysis. Second, the configuration is modified from a batch to a continuous vessel design. The continuous design employs a counter-current extraction through an inclined screw conveyor, where the biomass is conveyed up the screw flights against a caustic solution flowing down the reactor. As biomass exits the top of the unit, a screw press squeezes liquor out of the solids material, which is recycled back to the extractor, leaving biomass at a targeted 30% total solids content to be routed to mechanical refining. The caustic exits with the black liquor, which then is re-utilized downstream in base catalyzed deconstruction of the DMR liquor combined with residual downstream lignin solids.

This continuous counter-current operation is based on the concept of weak black liquor recycling across batch deacetylation cycles as published in Chen et al. [44]. In that cited study, proof-of-concept experiments found the ability to recycle the caustic solution in the weak black liquor across a number of batch cycles, each time increasing the strength of the black liquor and thus the concentration of acetate and solubilized lignin species (as well as other soluble solids) while generally holding carbohydrate losses constant into the liquor phase. This would prove beneficial as the single-batch deacetylation approach would yield a black liquor product too dilute for economical conversion through the lignin bioconversion step, but which cannot be concentrated either without re-precipitating the solubilized lignin components. With recycling of the liquor across multiple passes over the biomass, this both saves on makeup water demands and accordingly reduces the water content of the final black liquor product relative to other solubilized components (further discussion on this concept and its logistical considerations may be found in Chen et al. [44]). At commercial scale for processing a continuous biomass feed to the facility, the present design extrapolates the reverse-sequential batch concept investigated experimentally to employ a continuous counter-current solid-liquid extraction unit with squeezed liquor from the outlet solids recycled back through the extractor. Design and cost considerations for this unit are discussed below.

Based on preliminary NREL experimental data at the above-stated conditions, the concentrated black liquor product is projected to comprise 100% of the acetate, extractives, and protein components originally present in the delivered biomass, as well as 50% of the sucrose, 66% of the ash, and (importantly) 47% of the lignin. Of the total solubilized lignin, roughly 15% is estimated to be monomers (primarily p-coumaric, ferulic, and vanillic acids) and the remainder remains in oligomeric form, subsequently routed along with downstream residual solid lignin through base-catalyzed deconstruction under more severe conditions for further conversion to monomers (discussed later). Additionally, this step incurs losses of carbohydrates (which are targeted to be somewhat mitigated through the counter-current liquor recycling design), set at targets of 2% glucan, 10% xylan, and 30% arabinan solubilizations into the liquor product. Although these losses from the fuel train are higher than prior targets with milder deacetylation conditions employed for DDA pretreatment [10], these solubilized carbohydrates are still utilized for conversion to biomass and muconic acid through the lignin coproduct train downstream, and so are not lost in valorization potential altogether. The water content of the concentrated black liquor is estimated at roughly 66 wt%, at a pH of 8-9. The projections asserted here for this operation carry a degree of risk as this has not yet been tested experimentally at NREL in this continuous configuration, and thus represents an important area for future study to validate or refine the present assumptions.

The extracted solids material is dewatered through a screw discharger at the end of the counter-current alkaline extraction unit and routed to mechanical refining. The mechanical refining operations consist of a primary disc refiner and a secondary step such as a roller mill or low-consistency disc refining (either option is anticipated to provide comparable performance), which together require a power demand of 200 KWh per dry tonne of processed solids based on previous vendor guidance. This power demand was previously found to represent an optimum between mechanical disruption of the biomass versus reasonable biorefinery power costs [42], given that this is a power-intensive step (although it saves on heat/steam demands, which are required for DDA pretreatment). The resulting particle size exiting DMR is typically 200-300 microns on average. All pertinent parameters for the DMR pretreatment step are summarized in Table 2.

Table 2. DMR Pretreatment Conditions Applied in this Design ^a

Parameter	Current design
Deacetylation (mild alkaline extraction)	
Temperature	92 °C
Residence time	90 min
Total caustic (NaOH) loading	70 mg/g dry biomass
Net solubilized glucan to liquor (wt%)	2%
Net solubilized xylan to liquor (wt%)	10%
Net solubilized arabinan to liquor (wt%)	30%
Ash removal (wt%)	66%
Solubilized acetate (wt%)	100% (10 g/L)
Solubilized extractives (wt%)	100% (79 g/L)
Solubilized lignin (wt%)	47% (40 g/L)
<i>P-coumaric acid (wt% of solubilized lignin)</i>	10%
<i>Ferulic acid (wt% of solubilized lignin)</i>	4%
<i>Vanillic acid (wt% of solubilized lignin)</i>	1%
<i>Lignin oligomers (wt% of solubilized lignin)</i>	85%
Mechanical Refining	
Solids loading (wt%)	30%
Power demand (KWh/dry tonne processed biomass)	200

^a DMR parameters are generally based on NREL experimental data observed to date on DMR processing with batch deacetylation, but extrapolated to higher targeted black liquor concentrations and marginally lower carbohydrate losses targeted for counter-current deacetylation/alkaline extraction.

A small flash tank is also maintained following the DMR process, but flashes a much smaller amount of steam than in the DDA design. From there, the slurry is routed to enzymatic hydrolysis after being diluted with water as appropriate for the given hydrolysis design considered (discussed below).

3.2.3 Cost Estimation

The counter current deacetylation unit was costed based on a Braunschweigische Maschinenbauanstalt AG sugar beet cossette extraction unit [45, 46]. This unit is designed to withdraw liquid from the solid cossettes via a double conical screen and is sized based on the biomass solid flow rate. For the mechanical refining equipment, both the disc refiner and roller mill (here, based on a Szego mill [<https://www.szegomill.com/>]) were based on vendor cost quotations provided when NREL began investigating DMR pretreatment, requiring 8 and 11 units respectively at a purchase cost of roughly \$2.5 MM and \$580,000 per unit (2013\$). In all, Area 200 contributes roughly \$1.42/GGE and \$1.48/GGE to the MFSP for the acids and BDO cases, respectively, including deacetylation, mechanical refining, and conditioning. About 31% of this is attributed to capital cost with the remainder attributed to caustic and power.

3.3 Area 300: Enzymatic Hydrolysis and Hydrolysate Conditioning

3.3.1 Overview

In this area, pretreated biomass is sent through enzymatic hydrolysis to convert polysaccharides to monomeric sugars using cellulase and hemicellulase enzymes, followed by hydrolysate conditioning in the case of the acids pathway. For the BDO pathway, enzymatic hydrolysis employs NREL's historical design assumptions including a 24-hour continuous vertical vessel followed by standard batch saccharification reactors. The whole-slurry hydrolysate (including solids) is then cooled and subjected to batch fermentation in the same tanks, reflecting a similar strategy as prior ethanol

pathway models [2]. However, for organization purposes, the fermentation portion of the batch time and associated tankage volume is allocated to A500 while the hydrolysis portion is allocated to A300.

For the acids pathway, a more novel continuous enzymatic hydrolysis (CEH) operation is employed utilizing a series of saccharification tanks in sequence, with each connected to a microfiltration membrane through a pump-around loop to remove sugars as they are produced, thereby reducing feedback inhibition and improving hydrolysis kinetics. The remaining solids are routed to the next hydrolysis vessel to repeat the process. Enzymes initially lost through the microfilters are subsequently recovered through an ultrafiltration step on the combined sugar product stream. The CEH process is targeted to achieve upwards of 96% hydrolysis of carbohydrates to monomeric sugars, but requires more dilute operating conditions (generally below 10% total solids), thus the clarified hydrolysate must be re-concentrated in a vacuum mechanical vapor recompression (MVR) evaporator. The clarified, concentrated hydrolysate is routed to downstream fermentation. Both A300 process schematics are depicted in Figure 4.

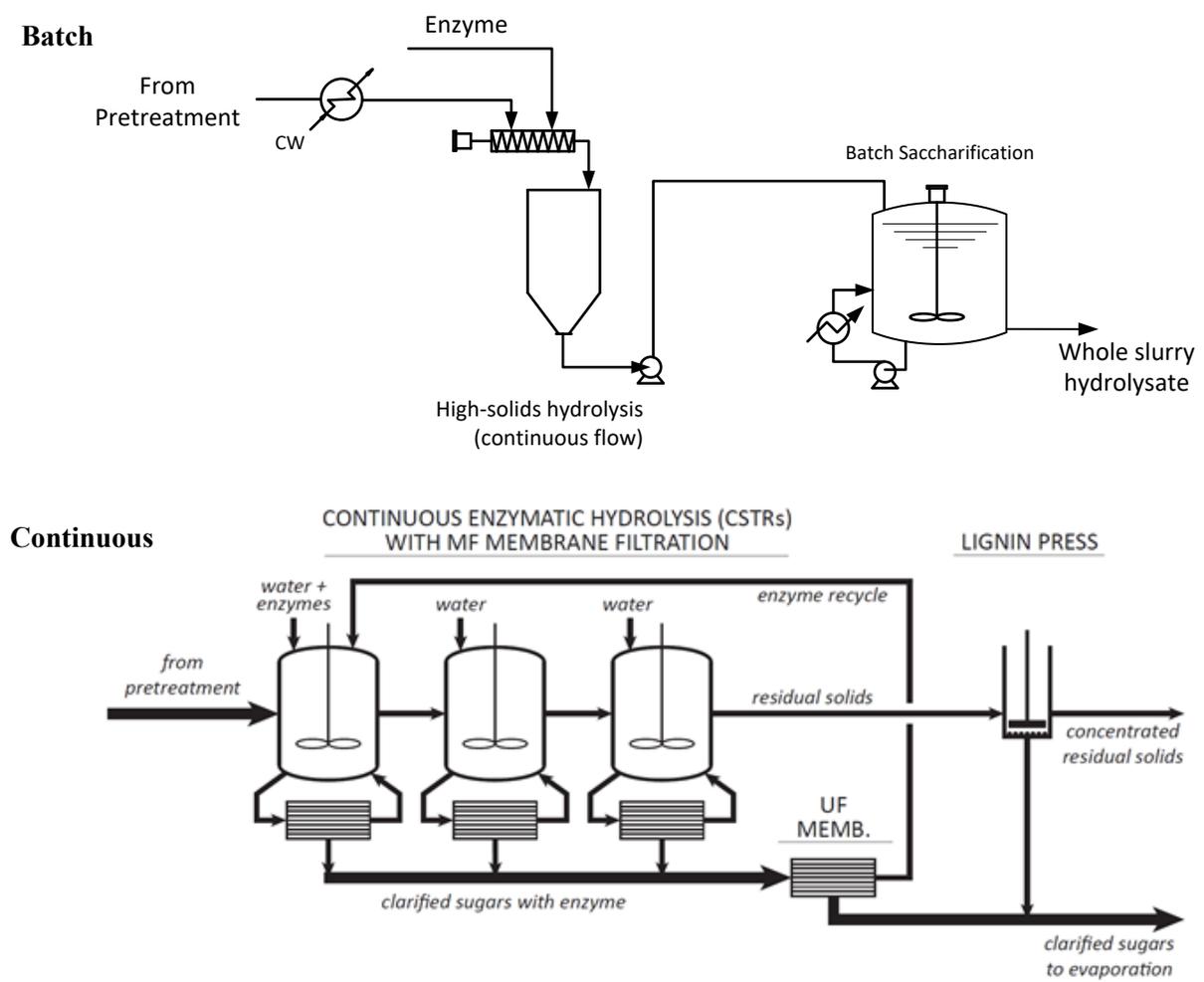


Figure 4. Process schematic diagrams for batch and continuous enzymatic hydrolysis/hydrolysate conditioning operations (BDO and acids pathways respectively)

3.3.2 Design Basis

BDO Pathway: Batch Enzymatic Hydrolysis

In the BDO case, the process and design basis for enzymatic hydrolysis is the same as described in the 2011 ethanol report and 2013 biological hydrocarbon report, thus will only be briefly summarized here. In short, enzymatic hydrolysis is initiated in a continuous, high-solids vertical tower reactor with the slurry flowing down the reactor by gravity; this first step is required as the feed material at 25% solids (or more) is not pumpable until the cellulose has been partially hydrolyzed. After mixing in the cellulase enzyme, the total solids loading into the continuous column reactor is 25 wt% and the temperature is 50°C (122°F). The residence time in the continuous reactor is 24 hours. After this point, the slurry is pumpable and is batched to one of eight 1 MM-gal vessels (950,000 gal working volume), where enzymatic hydrolysis continues for another 96 hours (5 days total hydrolysis time). The batch reactors are agitated and temperature controlled at 50°C using a pump-around loop with cooling water heat exchange. This represents a slight increase in hydrolysis temperature relative to prior design cases (48°C), based on experimental conditions more recently employed. When hydrolysis is completed, the hydrolysate is cooled and fermentation is initiated in the same vessels, discussed in Section 3.5. This is consistent with the sequential hydrolysis and fermentation (SHF) approach taken in the 2011 ethanol design case, but more recent review feedback suggested that this may pose a higher risk of contamination as the hydrolysate is cooled in the same tank for initiating fermentation. However, the alternative to send the hydrolysate to a heat exchanger and then a separate tank for fermentation would carry a minimal cost difference as the hydrolysis and fermentation vessels are the same and are sized/costed based on summative batch times for hydrolysis plus fermentation.

The amount of enzyme used (the enzyme loading) is still reported here based on the amount of cellulose present in the hydrolysate, even though the enzyme now must include both cellulase and hemicellulase activity given that hemicellulose was not substantially hydrolyzed upstream in DMR pretreatment as is achieved in DDA pretreatment. Total enzyme loading is targeted at 10 mg enzyme protein/g cellulose with a target of 90% conversion of cellulose to glucose and xylan to xylose, as well as 85% arabinan to arabinose. NREL's latest 2017 state-of-technology performance efforts demonstrated 78% glucan conversion and 85% xylan conversion to monomeric sugars at a 12 mg/g total enzyme loading on DMR substrates. Thus, the targets proposed here to be achieved by the year 2030 are not unreasonable projections given ongoing advancements in enzyme development. Directionally less enzyme is also needed than prior designs due to the reduction in active lignin deactivation sites given high upstream lignin removal. However, an additional risk is posed in continuing shifts to new feedstock blends rather than a single feedstock (corn stover), which may prove more recalcitrant to enzymatic hydrolysis. The target design conditions for enzymatic hydrolysis are summarized in Table 3.

Table 3. Standard Enzymatic Hydrolysis Conditions

Temperature	50°C (122°F)
Initial solids loading	25 wt % total solids
Residence time	5.0 days total (96 h)
Number and size of continuous vessels	6 @ 950 m ³ (250,000 gal) each
Number and size of batch vessels	8 @ 3,600 m ³ (950,000 gal) each
Total enzyme (cellulase + hemicellulase) loading	10 mg protein/g cellulose

Acids Pathway: Continuous Enzymatic Hydrolysis and Concentration

In the acids case, because acids fermentation includes circulation of the fermentor broth through a pertractive membrane for recovery of the acids, insoluble solids must first be removed to avoid clogging the membrane. This could be accomplished using a similar batch enzymatic hydrolysis step as for the BDO pathway, followed by a vacuum belt filter press with addition of a flocculant. However, this operation incurs significant costs for both the filter press capital expenses as well as the cost of the flocculant; filtration is also more challenging for DMR hydrolysate, requiring high flocculant loadings (at least 20 g/kg insoluble solids) at lower membrane permeances (at most 15 kg insoluble solids/m²-h) to achieve 95% sugar recoveries (as may be found in NREL's sugar model scenarios available from <https://www.nrel.gov/extranet/biorefinery/aspen-models/>).

Alternatively, recent NREL research has begun investigating the more novel continuous enzymatic hydrolysis approach wherein hydrolysis is initiated in a continuous stirred tank reactor (CSTR) vessel connected through a pump-around loop to a microfilter, which continuously removes sugars as they're produced while retaining the unhydrolyzed solids. This improves hydrolysis kinetics by reducing sugar feedback inhibition, allowing for lower hydrolysis volumes, higher sugar yields, and/or lower enzyme loadings based on NREL proof-of-concept experimental work at bench scale (3 L reactor volumes operated over 80 hours) [47]. The residual solids from one CSTR step are routed to a subsequent CSTR with the same setup, and this process is repeated several times (in this design, using three CEH reactors in series). Enzyme retention through the microfiltration units is not perfect, and "leaked" enzyme is captured and recycled through a subsequent ultrafilter located on the combined microfilter permeate streams. Prior TEA modeling for this concept demonstrated the potential for significant MFSP cost savings, on the order of \$1.50/GGE relative to a benchmark case employing batch enzymatic hydrolysis (EH) and vacuum belt filtration [12], albeit the reference case was based on older enzyme performance levels reflective of NREL's 2012 ethanol demonstration runs [40]. Relative to newer enzymes available currently (or moving into future years), at 90% projected sugar yields, the magnitude of MFSP savings would not be as large for CEH. However, with the projection of such yields for batch EH in the future, CEH is envisioned to improve on this further by achieving at least 96% conversions to monomeric sugars while maintaining the same 10 mg/g targeted enzyme loading.

It bears noting that this CEH concept carries a risk that is not yet well-understood, regarding the ability of all enzyme proteins to maintain a consistent composition over numerous recycles. Particularly given the use of both cellulase and hemicellulase enzyme cocktails in this design, different enzymes may have different levels of resistance to shear, oxidation, and denaturation across the multiple filtration and recycle steps, and different enzyme proteins may not be retained equally which may lead to a compositional imbalance in the cocktail mixture over time. This has not yet been investigated experimentally at NREL over longer-term trials and remains an area of future study, although it is known that different components have different binding characteristics and that binding affinities can be modified through protein engineering (an activity that NREL hopes to investigate in the future to reduce non-productive binding to lignin-rich residues).

While CEH can achieve improved hydrolysis yields, it also is limited to lower solids loadings because each stage is maintained at a consistent IS level after dilution with water (i.e., IS does not decrease over the course of the process as it does in batch EH). The operation is targeted at 7.5% IS loading (roughly 7.6% TS loading) as a maximum level constrained by CSTR agitation ability and pumpability through the membrane pump-around loops. Current experimental work has so far been done closer to 5% IS levels, but 7.5% is viewed by NREL researchers as a plausible future target. This more dilute

operation translates to high water content in the solids outlet stream from the final stage, roughly 87% moisture content, which is too high to be sent directly to the boiler. Thus, the original lignin press unit, as utilized in NREL’s 2011 ethanol case [2] for separating lignin from the ethanol beer stillage, is re-incorporated at this point to reduce water content of the solids stream to 35%, which also carries an additional benefit of recovering 95% of the sugars initially lost with the solids (thus translating to an overall recovery of 99% of all produced sugars across CEH). Over 90% of the water is also removed from the solids with the clarified sugars, with a minimal amount of water evaporated from air drying.

While the inlet and product water content of the solids across the lignin press is similar to the original conditions for that unit in the ethanol process, because the solids here are from DMR pretreatment, filterability across the lignin press will be more challenging, and may require the assistance of a flocculant (as is required for the vacuum filter press when processing the main hydrolysate stream). This is not yet well-understood but will be further considered in the future. The target design conditions for CEH are summarized in Table 4.

Table 4. Continuous Enzymatic Hydrolysis Conditions

Temperature	50°C (122°F)
Steady-state solids loading	7.6 wt % total solids (7.5% insoluble/0.1% soluble)
Number of CSTR stages	3
Stage residence time	30 hr – 53 hr – 71 hr
Total enzyme (cellulase + hemicellulase) loading	10 mg protein/g cellulose
Microfiltration permeance	100 kg/m ² /hr
Total microfiltration area	95,783 ft ² (8,898 m ²)
Ultrafiltration permeance	67 kg/m ² /hr
Total ultrafiltration area	114,940 ft ² (10,678 m ²)
Overall recovery of produced sugars	99%

The conversions taking place during both standard and continuous enzymatic hydrolysis are listed in Table 5. As noted above, because enzymatic hydrolysis must convert both cellulose and hemicellulose components to monomeric sugars given the use of DMR pretreatment, these sugar yields implicitly indicate a combination of both cellulase and hemicellulase activity for the total enzyme loading specified above.

Table 5. Standard and Continuous Enzymatic Hydrolysis Reactions and Assumed Conversions

Reaction	Reactant	% Conversion (Standard EH)	% Conversion (Continuous EH)
(Glucan) _n + n H ₂ O → n Glucose	Glucan	90%	96.3%
(Glucan) _n + n H ₂ O → n Cellobiose	Glucan	1.2%	0%
(Xylan) _n + n H ₂ O → n Xylose	Xylan	90%	98.8%
(Arabinan) _n + n H ₂ O → n Arabinose	Arabinan	85%	98.8%

The clarified filtrate exiting microfiltration and ultrafiltration from CEH is also fairly dilute at 5.5% sugars, and is thus pumped to hydrolysate concentration, consisting of a four-stage MVR evaporation system, which produces a concentrated sugar stream of 49% (monomeric) sugar, 50% water, and 1% other dissolved solids for downstream acid fed-batch fermentation. The 50% total solids specification is set as an estimated balance between evaporation cost, syrup viscosity, and downstream fermentation sizing/operation, but further room exists for optimization on this parameter in the future. Also by including hydrolysate concentration, this provides a more microbially stable stream for fermentation.

The evaporator design and cost basis is consistent with prior design reports [10]. To avoid the possibility of sugar degradation at high temperatures [48], the evaporators are assumed to be operated under slight vacuum to keep the maximum temperature below 90°C (194°F). The vapor exiting the evaporation system is nearly all water (approximately 99.9% purity) and can be recycled directly to the process water manifold after being condensed by water cooling. The vendor-provided evaporation system design specifications are summarized in Table 6.

Table 6. CEH Filtrate Evaporator Specifications

Feed sugar concentration	5.5 wt %
Product sugar concentration	49 wt % (50% water, 1% other solubles)
Maximum operating temperature	87°C
Evaporator technology	MVR
Number of effects	4
Electricity usage	14,454 KW (19,383 hp)
Steam usage (low-pressure steam)	1,550 kg/hr (0.8 MMkcal/hr)

3.3.3 Cost Estimation

For the BDO case utilizing the standard enzymatic hydrolysis operations, the design and cost basis assumptions for all hydrolysis equipment were left unchanged from prior design cases [2, 10], namely empty towers for the continuous hydrolysis reactor based on a vendor quotation for flat-bottomed plug-flow reactors with a 10:1 height to diameter ratio, as well as 1 MM-gal batch hydrolysis reactors and agitators. The material of construction for enzymatic hydrolysis equipment is 304SS. As noted above, after batch hydrolysis is complete, the hydrolysate is cooled and BDO fermentation is initiated in the same 1 MM-gal vessels; however, for cost tracking purposes, the portion of the batch time (4 days) and associated tankage volume (5.7 MM gal) attributed to hydrolysis is assigned to Area 300, with the remainder for BDO fermentation (1.5 days and 2.1 MM gal) assigned to Area 500.

For the acids case utilizing CEH, the CSTR vessels are costed consistently with the standard batch hydrolysis reactors noted above, using multiple 1 MM-gal vessels for each stage and thus costing the reactors based on total volume with a linear scaling factor. All membrane costs are based on subcontractor guidance for ultrafiltration membranes, with costs scaled linearly based on membrane area (calculated from the given permeance targets above). The original quoted cost basis was \$2.05 MM (2011\$) for a membrane area originally sized at 53,820 ft². This basis is applied for both the microfilter and ultrafilter membranes here, thus may err on the conservative side for the larger pore size microfiltration units, but allows for a safety factor in the costing for this more preliminary CEH concept. A provision was also included for an additional spare membrane unit in the event of membrane fouling/plugging or other required maintenance and membrane lifetime was assumed to be two years. The sugar concentration (MVR evaporation) equipment is also based on vendor-provided design and cost estimates, consistent with information provided in the 2013 design report [10].

3.4 Area 400: Enzyme Production

3.4.1 Overview

This process area produces cellulase and hemicellulase enzymes used in Area 300 to hydrolyze cellulose into glucose and xylan/arabinan into xylose/arabinose respectively. Cellulase is produced industrially using (among other microorganisms) *T. reesei*, a filamentous fungus that secretes high levels of cellulase enzymes when grown aerobically in the presence of cellulose or other cellulase

inducers. The present analysis maintains consistency with the fundamental assumptions for enzyme production and cost estimation as detailed in the 2011 ethanol report and 2013 biological hydrocarbon report, most importantly, the use of on-site enzyme production rather than a purchased-enzyme model. As stipulated in prior reports, we again note that by including an on-site enzyme production section, NREL and DOE are not making a judgment about whether or not the cellulosic biofuel industry should align to this mode of enzyme distribution. Rather, the model on-site enzyme section is intended to improve transparency in determining the true cost of cellulase enzymes for large-scale cellulosic biofuel production.

Consistent with earlier design cases, the present design considers submerged aerobic cultivation (“aerobic fermentation”) of a *T. reesei*-like fungus on a feedstock of glucose and fresh water. While hydrolysate could alternatively be used directly to cultivate the enzyme, the use of glucose likely enables higher enzyme titers and thus lower capital costs and utility demands. We have assumed a media preparation step where a small fraction of glucose is converted to sophorose, a powerful inducer of cellulase, using a small amount of the cellulase enzyme itself. When grown on this substrate, *T. reesei* has been shown to productively secrete cellulase [49]. It is noted that one difference in the present work is that both cellulase and hemicellulase enzymes are required in the enzymatic hydrolysis step, but the same overall enzyme production process framework is maintained, assuming the costs of producing a quantity of enzyme protein are similar whether for cellulase or hemicellulase. This may require two production host strains given practical limitations to the number of enzymes a single strain can express, but in that case if both strains could be co-cultivated in the same shared bioreactor configuration (i.e. did not require two parallel process trains), the overall TEA cost implications would be minimal. This assumption may be revisited in future work if further validation or guidance from industry is received. The whole broth product is transferred to the hydrolysis tanks without an enzyme isolation step. Figure 5 is a simplified flow diagram of the enzyme production section.

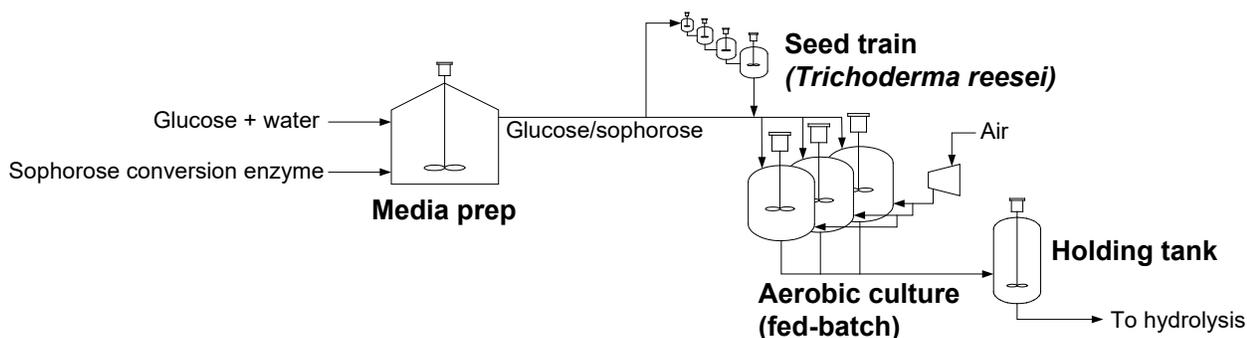


Figure 5. Simplified flow diagram of the enzyme production process

3.4.2 Design Basis

The design for the enzyme production operations is described in detail in the 2011 ethanol report and will not be repeated in such detail here. In summary, the design for the system was based in part on the claims in Example 5 of U.S. Patent 4,762,788 [50, 51] in combination with a number of reasonable assumptions to develop a rudimentary process as documented in the 2011 ethanol report. The key assumptions used in the current design are summarized in Table 7.

Table 7. Area 400 Guiding Design Basis Assumptions

Parameter	Assumption
Protein loading to enzymatic hydrolysis	10 mg protein/g cellulose
Reactor size	300,000 L @ 80% final working volume
Enzyme titer at harvest	50 g/L
Mass yield of enzyme from glucose	0.24 kg enzyme/kg glucose
Enzyme production cycle time	120 h online, 48 h offline, 168 h total

The targeted total cellulase and hemicellulase loading to enzymatic hydrolysis is set in the present pathway model to 10 mg of enzyme protein per g of cellulose as also assumed in the 2013 biological conversion report, down from 20 mg/g in the 2011 ethanol report, as described in Section 3.3. Here, “protein” refers to the total amount of high molecular weight protein in the enzyme broth as determined by assay; not all of this protein is active cellulase/hemicellulase. The total protein demand was thus calculated to be 260 kg/h (570 lb/h). An additional 10% is produced to account for the slipstream provided to the media preparation tank to make the glucose/sophorose mixture.

The size of the cellulase production vessels was set at 300 m³ (80,000 gal) with a height-to-diameter ratio of 2. Fermentation is assumed to be a fed-batch process starting at 50% working volume and ending at 80%. Over one week, each bioreactor will see a 24-hour cell growth period, a 96-hour protein production period, and a 48-hour offline period for draining, cleaning, and refilling. With a 1-week total cycle time and the production parameters listed in Table 7, one bioreactor is capable of producing 12,000 kg of protein in a week, or 71.4 kg/h (157 lb/h). The equivalent enzyme volumetric productivity is 0.30 g protein/L-h. Five production reactors were therefore required to deliver the 260 kg/h of protein needed for enzymatic hydrolysis. The reactors are loaded initially with the glucose/sophorose carbon source and nutrients, including corn steep liquor (CSL), ammonia, and sulfur dioxide (SO₂). After the initial cell growth period, additional substrate is added to maintain protein production. The bioreactors are sparged with compressed and cooled air and corn oil is added as antifoam. The reactors are temperature-controlled by chilled water flowing through internal coils.

Aeration and agitation requirements for the production bioreactors are functions of oxygen transfer rate (OTR) and oxygen uptake rate (OUR), which have been discussed in detail in the 2011 ethanol report and again in the 2013 report. Thus, the details and governing principles for these metrics will not be repeated again here. In the modeled bioreactors, the reaction stoichiometry balances the reactions of substrate, oxygen, ammonia, and SO₂ to cell mass and enzyme (plus CO₂ and water) using an elemental composition for commercial enzyme provided by Novozymes [51]. The composition of cell mass was taken as the average of a generic cell mass composition [52] and the enzyme composition, with the assumption that cell mass includes some unreleased protein.

Enzyme protein: CH_{1.59}N_{0.24}O_{0.42}S_{0.01}

T. reesei cell mass: CH_{1.645}O_{0.445}N_{0.205}S_{0.005}

In the production bioreactors, it is assumed that 90% of the carbon source is converted via the protein reaction and 10% is converted via the cell mass reaction. In the seed reactors, 85% of the carbon is converted via the cell mass reaction and 5% via the protein reaction, with 10% unreacted. This represents an overall molar selectivity of glucose to 31% protein, 4% cell mass, and 65% CO₂,

yielding 0.24 kg enzyme protein/kg glucose. The final specifications for the enzyme production reactors are shown in Table 8.

Table 8. Specifications of the Enzyme Production Bioreactors

Total volume	300 m ³ /80,000 gal
Maximum working volume	80%
Height-to-diameter ratio	2
Height	11.5 m
Diameter	5.75 m
Operating pressure	1 atm
Operating temperature	28°C (82°F)
Material	316SS
Agitator	800 hp
Total electricity demand per kg protein (air compressors, agitators, chillers, pumps)	9 KWh/kg

Four trains of three seed fermentors provide inoculum to the main enzyme production bioreactors. Each vessel in the seed trains is run batchwise on the same substrate as the production vessels. It is possible that by running in a semi-continuous fill-and-draw mode, the seed tankage volume and complexity could potentially be minimized to reduce the number of seed stages, but this has not been evaluated through dynamic process modeling and thus the standard three-stage batch operation is maintained. Air is also sparged through each of the seed vessels, which are cooled with chilled water. The seed bioreactors are each sized at 10% of the next stage volume, i.e., 0.3 m³, 3 m³, and 30 m³. The aeration demand is assumed to be 10% of the production aeration rate. Four trains were chosen because each production fermentor has a total cycle time of 7 days; each seed fermentor should have a cycle time of 2 days (including cleaning and sterilization) to get through the cell growth phase only.

Like the oxygen uptake rate, the glucose demand is also computed stoichiometrically from the required protein production rate. Ammonia and SO₂ are fed to the reactors stoichiometrically and CSL, trace nutrients, and antifoam (corn oil) are added to the substrate based on flow rate. The required nutrient concentrations are based on Schell et al. [53] and remain the same as presented in prior design reports. Glucose, the carbon source for cell mass and protein, is the most significant enzyme production expense in this model. The cost for glucose was updated to the latest five-year average price of glucose syrup, as discussed in Section 4.3. Electricity also remains a significant contributor due to the power requirements of air injection, agitation, and refrigeration. Total electricity demand for these operations is shown in Table 8.

3.4.3 Cost Estimation

The cost estimation for all equipment in A400 was left unchanged from the basis values provided in the 2011 ethanol report and maintained in the 2013 case, thus will not be repeated in detail here. Most equipment in this area is stainless steel. The air compressor and some of the nutrient delivery equipment items are specified as carbon steel. Quotes for the production bioreactors, internal cooling coils, production agitators and motors, skid-mounted seed fermentors, and air compressor were provided by vendors through Harris Group, which developed costs for the pumps in this area using their historical database. Not included in the enzyme production model are any costs for concentration, stabilization, or transportation of the enzyme to the plant, which would not be required in this case for on-site production. Whether for on- or off-site enzyme production, one expects to have to pay

licensing fees for the cellulase production microorganism, but that cost is not included as any amount would be speculative without availability of such licensing costs; however, a reasonable range is considered later in the Sensitivity Analysis section. The enzyme production system is also sized strictly to provide the amount of enzyme required for the hydrolysis step (e.g., is not oversized to accommodate occasional poor-yielding runs), reflective of the n^{th} -plant approach taken elsewhere in the design (e.g., avoiding over-design of equipment operations).

Based on the economics of the on-site enzyme section described above, the predicted cost of enzymes to the facility is roughly \$0.43/GGE of total fuel product in the acids case example. The resulting enzyme cost on a per-kg basis is \$6.16/kg protein in 2016\$. The caveat discussed in prior design reports bears repeating, that the enzyme cost contribution modeled here is lower than one would expect for an enzyme preparation purchased from a separate, non-adjacent production facility. Transportation of the enzyme to the biorefinery facility could add a non-trivial amount to enzyme costs, even if formulation costs could be avoided. Furthermore, by lumping the enzyme production equipment in with the biorefinery, some key items are inherently shared, e.g., the land and buildings, cooling tower, and utilities infrastructure. Overhead and fixed costs, especially labor and management, would also be higher for a standalone facility. Additionally, an external enzyme production facility would probably demand a higher rate of return than the 10% IRR assumed for the biorefinery plant because it is a higher-risk and lower-volume business. Still, in the near term it is more likely that cellulosic biorefineries (whether targeting sugars, ethanol, or hydrocarbons) will purchase enzyme from an external supplier with an organization dedicated to improving enzyme performance and reducing costs.

3.5 Area 500: Fermentation, Catalytic Conversion, and Upgrading

3.5.1 Overview

Area 500 includes all core processing steps for conversion of the liberated sugars to hydrocarbon fuels/blendstocks via biological conversion to intermediate fuel precursors and catalytic upgrading of those intermediates to finished products. Both bioconversion pathways are anaerobic as introduced previously and further rationalized below.

In the BDO pathway, after batch enzymatic hydrolysis is completed, the hydrolysate is cooled and batch fermentation is initiated in the same vessels. BDO fermentation utilizes an engineered strain of *Zymomonas mobilis* to convert sugars to 2,3-BDO plus hydrogen as a byproduct for achieving cell redox balancing (the latter is purified from the fermentation off-gas and used downstream to help meet catalytic upgrading hydrogen demands). The fermentation is conducted on whole-slurry hydrolysate with the presence of solids, targeted here at 25% total solids. The fermentor product broth is routed to a lignin press to remove solids, and then to a polishing filter to remove particle fines and ion exchange to mitigate ionic/salt species that may be problematic for the downstream catalyst. The aqueous BDO stream is then heated at elevated pressure and routed to catalytic BDO upgrading, producing butene and minor byproducts. The butene product is distilled from water and upgraded to oligomers in the C8-C16 range, and then finally sent through a hydrotreating step to saturate the oligomers to paraffinic hydrocarbons.

In the acids pathway, the clarified/concentrated hydrolysate is routed to anaerobic fermentation using *Clostridium tyrobutyricum* to produce butyric acid, which is continuously removed as it is produced through a pump-around loop connected to an extractive membrane (pertraction) system. The acid

passes through the membrane into a solvent phase, then is sent to distillation to recover and recycle the solvent. Similar to the BDO pathway, the acid fermentation step also co-produces hydrogen, which is purified from the off-gas and used to help satisfy biorefinery hydrogen demands downstream. The recovered acid is then catalytically upgraded through a ketonization step to (primarily) 4-heptanone and CO₂, with the latter flashed off and routed to a scrubber to recover volatilized ketone. Next, the material is upgraded across a condensation step to an oxygenated C14 component in the presence of a solvent (subsequently distilled and recycled), and finally routed through hydrotreating to remove oxygen, leaving an isomerized C14 hydrocarbon for use as a diesel blendstock. The key unit operations for both pathways are shown schematically in Figure 6.

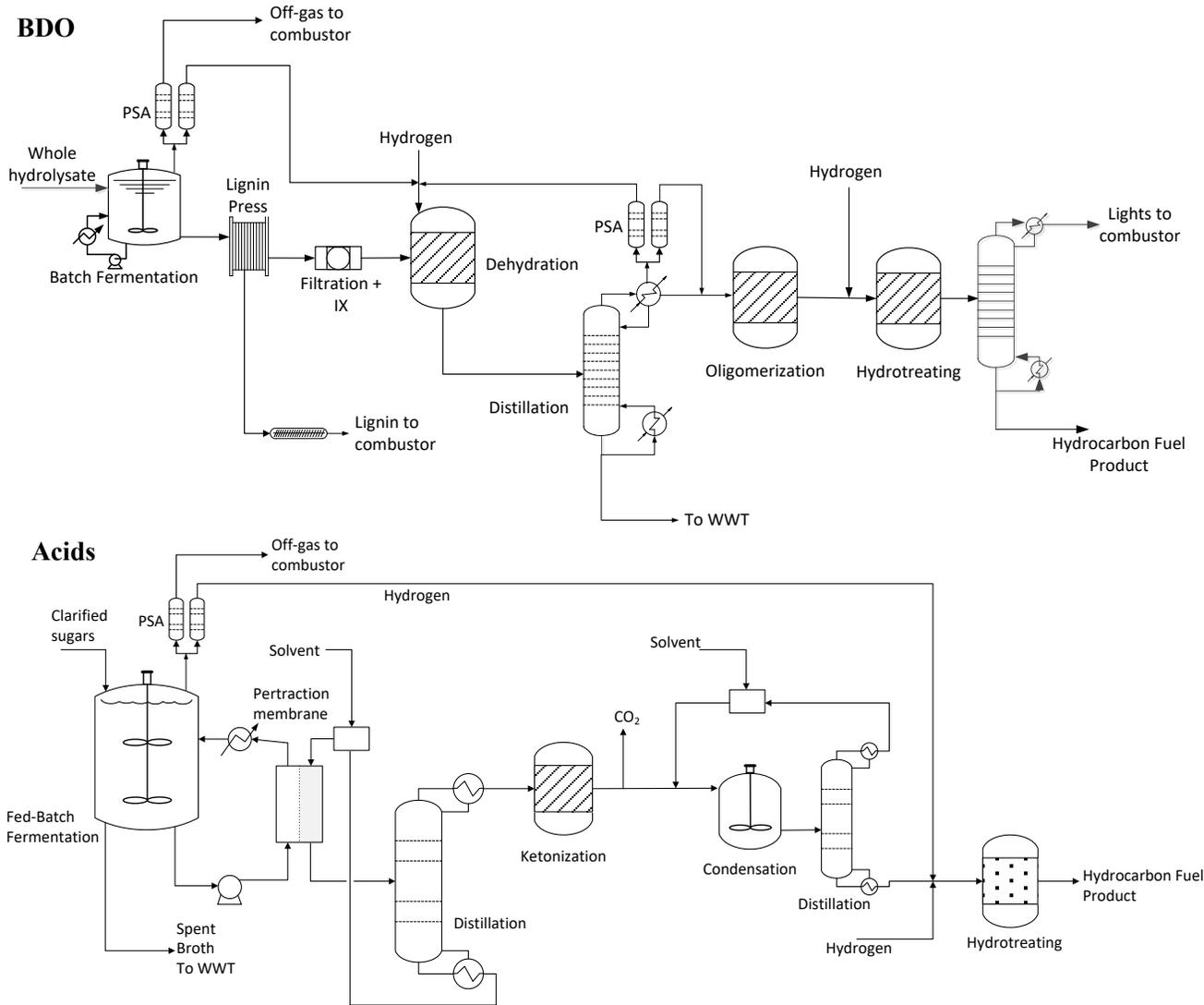


Figure 6. Simplified flow diagram of the fermentation, catalytic conversion, and upgrading process for both fuel train pathways

3.5.2 Design Basis

Anaerobic Fermentation: Background Context

As introduced in Section 1.1, compared to anaerobic fermentation, aerobic bioconversion is constrained by higher costs for oxygen delivery, both for the equipment to compress and sparge air into the bioreactor media, as well as associated power demands for compression and cooling demands for removing more evolved heat [13]. However, more significant factors are the economy-of-scale penalties for significantly smaller bioreactor volumes (500–1,000 m³ as required for maintaining uniform concentrations of dissolved oxygen and more stringent control of fed-batch fermentations), compared to anaerobic batch bioreactors on the order of 1 MM gal (roughly 4,000 m³) [54, 55]. This translates to 4–8 times more bioreactors required for aerobic versus anaerobic fermentation. While access to industry information is sparse with respect to maximum anaerobic fermentor vessel size possible, 1 MM gallon stirred tank vessels are commonly implemented in corn and cellulosic ethanol commercial facilities (feedback from industry).

These drivers contribute to an MFSP premium on the order of \$2/GGE for aerobic bioconversion options for sugars-to-hydrocarbon pathways relative to anaerobic options, as presented earlier in Figure 1. This economy-of-scale penalty translates to a stronger influence of fermentation capital costs for aerobic pathways, which in turn is dependent on achievable fermentation productivity as reflected in Figure 7, with aerobic yeast lipid productivity targets previously set at 1 g/L-hr. NREL's latest TEA efforts on aerobic bioconversion assumed the use of 1,000 m³ bubble column bioreactors, which correspond to the largest aerobic bioreactor systems currently deployed commercially; however, recent feedback from a consultancy with Genomatica indicated that potentially up to 2,000 m³ sizes may still be plausible as *n*th-plant designs for commodity production (thus shrinking economy of scale differences to within 2X versus anaerobic) [56]. Such large sizes would in fact exacerbate dissolved oxygen variations throughout the reactor, but Genomatica noted that this would not necessarily be insurmountable given sufficient strain development.

Beyond the aerobic cost challenges, the most developed/straightforward pathway that had previously been the primary focus of NREL's (and others') research—intracellular production of lipids via oleaginous yeast—also faced a significant risk in the ability to demonstrate lipid secretion, or at a minimum cell autolysis, as a key future goal in order to avoid significant costs incurred for cell disruption and intracellular lipid extraction. If this goal were not achieved, our TEA estimated an *additional* cost penalty on the order of roughly \$1.50/GGE (Figure 7), which would be insurmountable in the ability to ultimately achieve under \$2.50/GGE final MFSP targets. While there is limited literature information indicating some success having been achieved for secretion of fatty acid derivatives [57, 58], this is generally viewed as a higher-risk hurdle given NREL's latest state of experimental efforts.

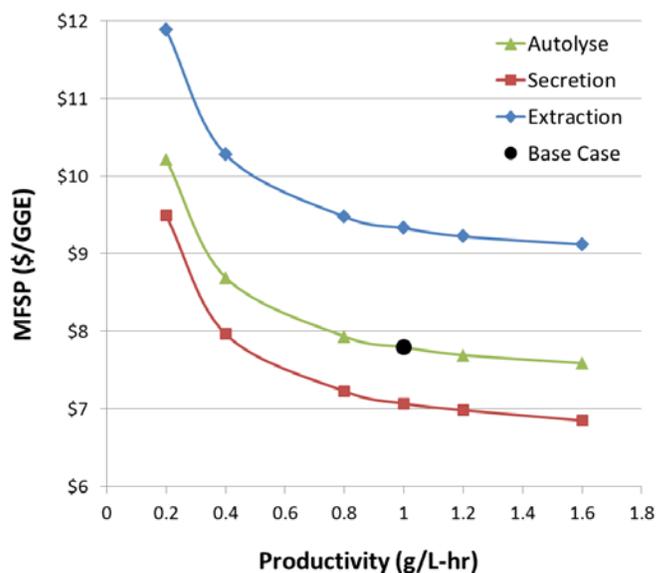


Figure 7. Scan plots for MFSP sensitivities to bioconversion productivity and product recovery method for aerobic lipids pathway (excluding lignin coproducts to reduce MFSP goals per top bars of Figure 1)

To further understand TEA ramifications for aerobic systems, more sophisticated models were built beyond the capabilities in Aspen Plus. Namely, the complex dynamics of operating an aerobic fed-batch bubble column with distinct phases for organism biomass growth versus lipid accumulation (and associated demands for OURs, OTRs, and nutrient feeding strategies) are challenging to accurately reflect in a steady-state process model framework like Aspen Plus. Accordingly, with assistance from an industry collaborator, a new model was built using Aspen Custom Modeler (ACM), which is an equation-based model that enables tracking such dynamic interactions based on engineering equations for oxygen solubilization coupled with a “black-box” metabolic model for oxygen uptake and cell/lipid accumulation (manuscript in preparation).

While the details and the mechanics of the ACM model are beyond the scope of focus for this report, to summarize the findings, a number of scenarios were investigated (Figure 8), including:

- a) Validation of prior Aspen Plus TEA estimates for a target case asserting cell autolysis of oleaginous yeast for low-cost lipid recovery (red versus pink curves in Figure 8, under a more narrow range of productivities as considered in Figure 7)
- b) Secretion of lipids from the cell under semi-continuous (rather than semi-batch) operation, either with diauxic or simultaneous metabolism of C6 versus C5 sugars (orange curves)
- c) Secretion of lipids under semi-batch operation with inclusion of cell recycle back to the bioreactor (lessening the diversion of hydrolysate carbon to new biomass growth; blue curve)
- d) Secretion of lipids under semi-batch operation with cell recycle, coupled with increased theoretical metabolic yields under a longer-term future scenario with a highly engineered cell (green curve).

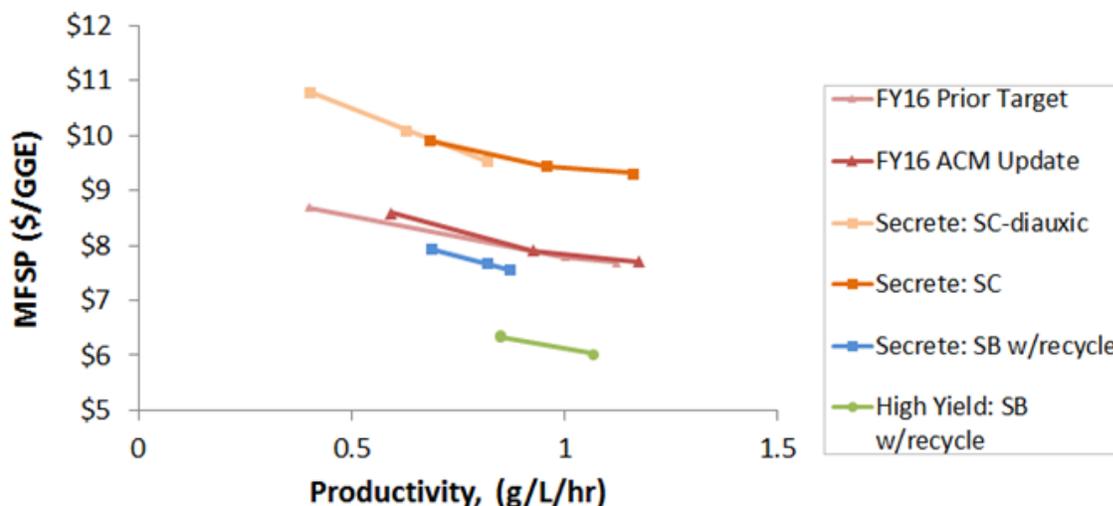


Figure 8. ACM model integrated with Aspen Plus TEA for investigation of aerobic lipid pathway scenarios. SC = semi-continuous; SB = semi-batch; recycle = incorporating cell recycle back to bioreactors to minimize carbon diversion from hydrolysate to grow new cell biomass; high yield = increased theoretical metabolic yields to lipids as implied in [59]. All cases prior to inclusion of lignin coproducts to reduce MFSP targets per top bars of Figure 1.

In short, the ACM model was found to confirm similar MFSP estimates as the steady-state Aspen Plus framework, thus further supporting the conclusions drawn around the “aerobic versus anaerobic” TEA tradeoffs discussed above. The ACM model also identified potential paths to further reduce MFSPs, most dramatically under case (d) above, nearly to a level comparable with the anaerobic pathway MFSPs shown earlier in Figure 1, albeit under a combination of targets that would likely require a longer-term research path than what could be more readily achieved under anaerobic fermentation approaches. Thus, for these reasons, the decision was made to focus on the anaerobic pathway options for fuel production in this design case (discussed below).

This is *not* intended to imply a universal recommendation against aerobic bioconversion in all instances, as many pathways for products, including high-value bioproducts, are inherently aerobic and their processing economics may likely support the higher values garnered by such products relative to commodity fuels. Indeed, both the enzyme train as well as the lignin coproduct train for this design case include aerobic bioconversion steps. Further, while NREL research targets had previously been set at 1 g/L-hr productivity goals for aerobic lipid production, this goal was subsequently achieved earlier than anticipated in 2017, implying further room likely would exist to continue improving on this moving forward into the future (recent industry feedback indicated performance on the order of 2 g/L-hr for certain anabolic products), although moving beyond the 1 g/L-hr level would lead to diminishing economic returns as shown in Figure 7. It is also noted that with the onset of advanced genetic engineering strategies “aerobic” is no longer a universally black-and-white distinction from anaerobic; pathway modifications and redox balancing can enable sizable reductions in oxygen demand compared to the native pathways and promote efficient conversion with very little oxygen [60].

Fermentation/Product Recovery: BDO

The anaerobic xylose and glucose fermenting bacterium *Z. mobilis* can be engineered to redirect carbon from ethanol to produce other products, but still take advantage of its high specific sugar uptake rate, rapid catabolism, and high carbon yield [14]. NREL initiated this effort starting in 2015 by recruiting three genes encoding acetolactate synthase, acetolactate decarboxylase, and butanediol dehydrogenase from *Enterobacter cloacae* to channel pyruvate to acetolactate, acetoin, and then to 2,3-BDO into *Z. mobilis*. 2,3-BDO production was demonstrated to reach a titer over 10 g/L in 2015 [61], and then 23 g/L in 2016 [62] from 10% glucose in lab medium under low oxygen conditions. At that time, the engineered *Z. mobilis* strain exhibited a yield from glucose for 2,3-BDO, alongside acetoin and ethanol coproducts, at 96% of theoretical. In 2017, NREL researchers demonstrated a BDO titer above 40 g/L from 10% glucose and also 42 to 48 g/L from glucose and xylose in DMR hydrolysate by knocking out the pyruvate decarboxylase (*pdh*) gene in *Z. mobilis* strain BC21 and eliminating ethanol production [63].

At present, BDO fermentation experimental work has maintained the use of minimal air intake to the bioreactor (whether by sparging or intake to the headspace) to provide some dissolved oxygen for purposes of organism redox balancing. The minimal aeration level for this purpose is not the same as aerobic fermentation and may be met by merely maintaining oxygen in the fermentor headspace (as has already been demonstrated experimentally). Thus, even if minimal oxygen was still required moving forward, it is expected that the same 1 MM-gal CSTR vessels could be maintained for this pathway (rather than the smaller aerobic bubble column designs and associated economic penalties discussed previously), potentially with minor modifications to ensure proper air supply to the headspace or higher agitation power demands. However, ongoing research efforts are working to engineer the organism to provide the necessary redox balancing in a different way, including co-production of hydrogen or succinic acid while eliminating oxygen requirements. Co-producing hydrogen while maintaining the same BDO yield would result in marginal cost savings but this modification can mitigate concerns with oxygen requirements in transforming this pathway from a microaerophilic to an anaerobic process. Thus, this modification is targeted as the basis for the projected design case here. Hydrogen is recovered from the fermentor off-gas at high purity via pressure swing adsorption (PSA) for both this and the acids pathway. Any safety apparatus requirements pertinent to this operation (i.e. explosion mitigation measures) are outside the level of granularity in cost estimations performed here, and are assumed to be included in equipment indirect cost factors.

The biological conversion of sugars to BDO can be performed on whole-slurry hydrolysate without the necessity of solid-liquid separation before fermentation. Also, *Z. mobilis* tolerates a higher concentration of BDO (>100 g/L) than ethanol [14], which enables the higher TS loading to be targeted here at 25% TS through enzymatic hydrolysis and fermentation to achieve such an elevated BDO titer (modeled here at 97 g/L given the targeted conversions and the 25% TS loading level). This also reduces energy usage and capital expenses for removing water downstream. The process targets overall sugar utilizations of 95%, 90%, and 85% for glucose, xylose, and arabinose, respectively (as well as 95% utilization of the biomass sucrose), translating to a targeted process yield of 0.47 g BDO/g total sugars, over a 1.5-day fermentation batch time and 32°C fermentation temperature.

Beyond the main fermentation step, the assumptions for seed train design and conversions are maintained consistently with the details discussed in the 2011 ethanol report (utilizing another strain of *Z. mobilis*), including a 10% split of hydrolysate to inoculum growth consisting of two trains of five

reactors each, increasing in size up to 200,000 gal (757 m³) operated in 24-hour batch cycles [2]. Nutrients for all fermentation and inoculum steps are also maintained with prior design cases, represented by corn steep liquor (CSL) and diammonium phosphate (DAP). During peer review of this report, it was noted that in 2017 the use of CSL disqualified advanced biofuel facilities from claiming Renewable Identification Number (RIN) credits. While this study does not include RIN credit considerations in the TEA calculations, we note that alternative nutrient sources (e.g. ammonia) are also possible, and either way would not constitute sizeable contributions to overall fuel selling price at the minimal levels they are utilized here. Additionally, given that the fermentors are not designed for aseptic operation, the same assumptions for contamination losses are maintained as in prior biological design cases, namely 3% loss of all sugars to lactic acid. All key BDO fermentation conditions and parameters are summarized in Table 9 and Table 10.

Table 9. BDO Fermentation Conditions

Organism	Recombinant <i>Z. mobilis</i>
Temperature	32°C (96°F)
Initial fermentation solids level	25% total solids
Residence time	1.5 days (36 h) = 2.6 g/L-hr productivity
Total BDO fermentation volume required	30,000 m ³ (7.9 MM gal)
Number and size of vessels allocated to fermentation	8 @ 3,600 m ³ (950,000 gal) each
Inoculum level	10 vol%
Corn steep liquor (CSL) level	0.25 wt%
Diammonium phosphate (DAP) level	0.33 g/L fermentation broth (whole slurry)
Inoculum production: number of seed trains	2
Inoculum production: number of batch stages	5
Inoculum production: maximum stage volume	200,000 gal (757 m ³)

Table 10. BDO Fermentation Reactions and Assumed Conversions

Reaction	Reactant	% Converted to Product
BDO Production:		
Glucose → 2,3-BDO + H ₂ + 2 CO ₂	Glucose	95.0%
Glucose + 0.047 CSL ^a + 0.018 DAP → 6 <i>Z. mobilis</i> + 2.4 H ₂ O	Glucose	2.0%
Glucose + 2 H ₂ O → 2 Glycerol + O ₂	Glucose	1.0%
6 Xylose → 5 2,3-BDO + 5 H ₂ + 10 CO ₂	Xylose	90.0%
Xylose + 0.039 CSL + 0.015 DAP → 5 <i>Z. mobilis</i> + 2 H ₂ O	Xylose	1.9%
3 Xylose + 5 H ₂ O → 5 Glycerol + 2.5 O ₂	Xylose	0.3%
Xylose + H ₂ O → Xylitol + 0.5 O ₂	Xylose	0.1%
6 Arabinose → 5 2,3-BDO + 5 H ₂ + 10 CO ₂	Arabinose	90.0%
Arabinose + 0.039 CSL + 0.015 DAP → 5 <i>Z. mobilis</i> + 2 H ₂ O	Arabinose	1.9%
3 Arabinose + 5 H ₂ O → 5 Glycerol + 2.5 O ₂	Arabinose	0.3%
Seed Train:		
Glucose + 0.047 CSL ^a + 0.018 DAP → 6 <i>Z. mobilis</i> + 2.4 H ₂ O	Glucose	4%
Xylose + 0.039 CSL + 0.015 DAP → 5 <i>Z. mobilis</i> + 2 H ₂ O	Xylose	4%
Overall BDO process yield (metabolic yield), g/g sugars		0.47 (0.45)

^a CSL and DAP are both nitrogen sources required for *Z. mobilis* growth. The stoichiometry shown above is only used to balance the compositions assumed for *Z. mobilis* cell mass.

Following completion of the fermentation batch cycle, the fermentor broth is routed to a clarification step, employing a lignin press to remove lignin and other residual solids, utilizing consistent assumptions as the 2011 ethanol design report for this operation as was used to clarify ethanol beer

stillage [2, 64, 65]. This step achieves 98% removal of insoluble solids and reduces water content in the solids material from 80 to 25 wt%; however, it also incurs a small 3% loss of BDO product. The majority of the *Zymomonas* biomass is also removed here, which is routed to the boiler and incinerated (as necessary for engineered organism destruction). Similar to the use of the lignin press on the CEH solids stream as discussed above, again it is noted that the nature of DMR-pretreated solids in the present design will make for more challenging filterability through the lignin press (versus DDA pretreatment), and could require the use of a flocculant to achieve reliable operation. As this is not yet well-understood, this will be an important area for further evaluation moving forward.

Catalytic Upgrading: BDO

Following bulk solids removal from the lignin press, the clarified BDO fermentation broth is further purified across a polishing filter (microfilter) to remove particle fines, followed by ion exchange to remove soluble cations and anions that may otherwise deactivate downstream catalysts. These operations were included here based on subcontractor guidance during NREL's 2015 catalytic upgrading design case focused on catalytic aqueous phase reforming of sugars to fuels [9], where they were deemed necessary to ensure catalyst protection at least in the context of those reactor systems. It is not well-understood whether such operations are also required here for aqueous BDO upgrading, but they were conservatively maintained using consistent design and costing assumptions as employed in the 2015 case. The polishing filter consists of parallel crossflow microfiltration skids with a pore size of 0.1 micron. The filtrate is routed to ion exchange for further purification. A separate-bed ion exchange system is utilized to remove a range of ionic species. Two resin bed trains are included—one for anions and one for cations [66]. There are two units installed in parallel to allow for regeneration of the resin, which is assumed to be required every 17 hours [66]. Resin is regenerated with acid and caustic. While specific components expected to be most problematic for downstream catalysts and their concentration limits are not known, it is expected that a separate-bed system utilizing both anionic and cationic resins will be sufficiently flexible to remove a wide variety of ionic impurities as required for downstream catalyst protection. An additional 1% loss of BDO is assumed across the combination of these two purification steps. The purified stream is then routed to BDO upgrading.

The 2,3-BDO product may undergo catalytic upgrading either based on high-purity or bulk aqueous catalysis. In the former case, there are several options for separating 2,3-BDO from fermentation broth, including traditional or more novel distillation techniques (i.e., reactive or membrane distillation), aqueous two-phase reforming, *in situ* recovery, integrated solvent extraction and pervaporation, steam stripping, reaction with formaldehyde, and vacuum membrane filtration [67, 68]. Standard distillation is the most straightforward approach for handling pertinent separations, but incurs significant energy penalties as the boiling point of 2,3-BDO (roughly 180°C) is higher than that of water, thus would require boiling all the water off from BDO [69]. To alleviate this, the liquor may first be concentrated by a vacuum evaporator to remove some of the water, which could be driven by power rather than heat for this step if utilizing an MVR evaporator. Subsequently the concentrated stream would be sent through two sequential distillation towers to separate and purify 2,3-BDO from the remaining water and residual soluble solids. The final BDO product (>92%) could then be catalytically upgraded to butenes or butadiene (e.g., using $\text{CsH}_2\text{PO}_4\text{-SiO}_2$ catalyst). Overall, this would be a highly energy-intensive option.

Alternatively, aqueous catalytic upgrading could use the full clarified fermentation broth directly without BDO purification. This approach could simplify the overall process concept by eliminating the BDO concentration/distillation steps noted above, although still would require heating (albeit not

boiling) the aqueous stream up to reaction temperatures and processing a larger aqueous throughput through the BDO upgrading reactor. Oak Ridge National Laboratory (ORNL) reported a technology converting ethanol and ethanol-water mixtures to hydrocarbon fuels over zeolite-based catalysts, which were shown to be robust in tolerating water content between 5 wt% and 95 wt%, as well as volatile impurities in the feed stream [70].

More recently in 2017, preliminary catalytic upgrading experiments were performed by ORNL researchers as proof-of-concept for similar aqueous conversion of diols, with similarly effective conversion using core-shell $\text{SiO}_2@\text{ZrO}_2$ catalysts. The products from this aqueous catalytic reaction were a mixture of butenes, methyl ethyl ketone (MEK), butadiene, C2–C3 olefins, 2-methyl propanal, acetone, and other minor components. The butene product would still require purification prior to subsequent oligomerization reactions but poses an easier separation since all products at that stage boil lower than water. This aqueous BDO upgrading approach is the basis considered in the present design configuration, based on inputs provided by ORNL collaborators for target projections on BDO fermentor broth [71].

Catalytic upgrading of 2,3-BDO to olefins involves cascade reactions, such as dehydration, hydrogenation, rearrangement, and other side reactions. Dehydration of 2,3-BDO leads to MEK and 1,3-butadiene. Rearrangement and dehydration reactions produce 2-methyl propanal. Product selectivity between these dehydration intermediates depends primarily on the type of acidic catalyst. Selective hydrogenation of carbonyl and 1,3-butadiene while maintaining olefins is challenging. Metal catalysts with mild hydrogenation properties (e.g. Cu) are needed this type of selective reaction. Bifunctional catalysts with dehydration and hydrogenation activity are key for one-step upgrading of 2,3-BDO to olefins (Figure 9). Depending on the type of catalyst employed, other side reactions are possible, such as coupling of butenes and cracking reactions.

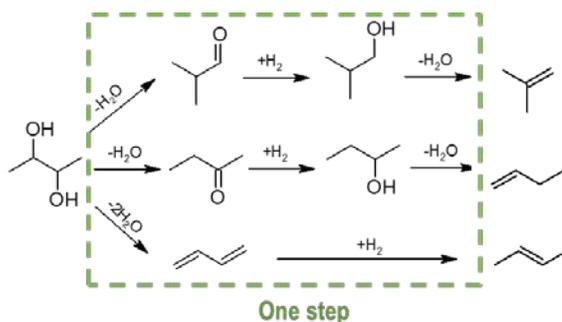


Figure 9. 2,3-BDO upgrading reaction pathways to olefins

For 2,3-BDO aqueous catalytic upgrading, bifunctional solid acid catalysts are used. In the present design, the aqueous BDO stream containing roughly 8 wt% BDO, 91 wt% water, and 1 wt% other components (primarily unconverted sugars) is converted adiabatically to dehydration intermediates over copper-based catalysts (e.g., $\text{Cu}/\text{SiO}_2\text{-ZrO}_2$ and $\text{Cu}/\text{zeolite}$) at 250°C and 45 atm [64, 65, 72]. As shown in Table 11, 100% of the BDO is converted to a number of representative components, namely butenes, pentenes, hexenes, MEK, and other minor C2–C3 components. Stoichiometric element balances are closed with hydrogen consumption and water formation, with model convergence based on the NRTL property package given the presence of oxygenated/polar components (this is the default property package in most of the biochemical model steps for both fuel train pathways).

The composition of products is dependent on the composition of the feed stream, the reaction temperature and pressure, space velocity, hydrogen/BDO ratio, and catalyst type. When the temperature decreases to 200°C, the selectivity of C3+ olefins drops to 60% while MEK approaches 40%. Space velocity also has a dramatic effect on the product selectivity. When weight hourly space velocity (WHSV) increases from 0.5 to 5.0 h⁻¹, C3+ olefins selectivity decreases and MEK selectivity increases.

Aside from this information, data in the public domain remains scarce on the topic of aqueous catalytic upgrading of 2,3-BDO to hydrocarbons, particularly in the context of biomass hydrolysate fermentation broth. Moving forward, to achieve the design case targets, continued focus on designing active and robust catalysts for aqueous BDO conversion at high selectivity will be important, as well as understanding (and if needed, minimizing) the impact of impurities in BDO fermentation broth on catalyst performance.

Table 11. Product Distribution of the 2,3-BDO Upgrading Reaction (Future targets at high conversion and selectivity to desired alkenes)

	Group	C percent, mol%	Product mol%	Yield mol%
Propene	C3	9.78	3.26	4.45
1-butene	C4	8.13	2.03	2.78
cis-2-butene	C4	14.83	3.71	5.06
trans-2-butene	C4	25.53	6.38	8.72
n-pentene	C5	13.20	2.64	3.61
n-hexene	C6	3.80	0.63	0.86
Propane	C3	1.36	0.45	0.62
Water	H ₂ O		48.28	65.93
Isobutane	C4	0.87	0.22	0.30
Isobutylene	C4	15.60	3.90	5.33
MEK	C4	6.88	1.72	2.35

The 2,3-BDO upgrading reactor cost is based on the aqueous phase reforming (APR) reactor in NREL's 2015 catalytic upgrading design case [66], sized based on the total aqueous flow rate into the reactor. The reactor operation consists of packed-bed pressure vessels, clad in 317L SS, and includes internals that support the catalyst and distribute the process fluid. Hydrogen is added to the reactors at a hydrogen-to-BDO ratio of 7.2 (molar basis). This reaction is assumed to convert near 100% of the 2,3-BDO (and/or ethanol if needed), with a WHSV of 2.0 hr⁻¹ and biannual catalyst replacement. The key reaction parameters are summarized in Table 12. Costs for this and all catalysts are presented in Section 4.3. As discussed previously, catalyst performance can be sensitive to a number of impurities that could pose challenges to catalyst lifetime, such as sulfur, cations, anions, solids, and coke [73]. The effect of remaining substrates (depending on the concentration) on the catalyst stability should be further evaluated in the future R&D work. A challenge for aqueous BDO upgrading is catalyst stability in the condensed water phase (acid catalyst support and metal leaching).

Table 12. 2,3-BDO Catalytic Upgrading Reactor Conditions

<i>Parameter</i>	<i>Operating Condition</i>
Hydrogen Molar Ratio	7.2 mol H ₂ /mol BDO feed
Operating Temperature	250°C
Operating Pressure	45 atm
WHSV	2.0 hr ⁻¹
Catalyst Type	Copper-based catalysts Cu/SiO ₂ -ZrO ₂ , Cu/zeolite
Catalyst Lifetime	2 years

The product of the BDO catalytic upgrading step is sent to distillation to remove water. The distillation is more straightforward for butene, which is a gas at ambient conditions, versus purification of BDO, which boils above water as noted previously. The other olefin products from BDO upgrading also boil lighter than water. Heat integration is done by cross-exchange between the hydrodeoxygenation (HDO) reactor feed and the butene distillation column bottoms product. A trim heater is placed after this exchanger on the BDO feed line to further heat the BDO stream to the reactor inlet temperature of 250°C.

The butene column overhead product containing the olefin components is routed through oligomerization to C₈–C₁₆ oligomers. The oligomerization step is modeled using a fixed bed reactor operated at 150°C and 15 atm, containing Amberlyst-36 resin at a cost of \$71/lb (2014\$), with a target WHSV of 1 h⁻¹. The butenes are oligomerized with a 28%, 63%, and 9% selectivity to butene dimers (C₈), trimers (C₁₂), and tetramers (C₁₆), respectively [74]. Pentene and hexene are oligomerized to dimers (C₁₀ and C₁₂). The conversions of propene and butene are assumed to be 95% based on literature data [75-77], while the conversions of C₅ and C₆ olefins are assumed to be 100% in the same oligomerization reactor. In the future, the oligomerization reaction conditions and product distributions may be refined as further inputs/data from bench experiments become available. The oligomerization is designed and priced as a pressurized reactor vessel with fixed beds for Amberlyst-36 resin catalysts. The key parameters for the oligomerization step are summarized in Table 13.

Table 13. Oligomerization Reactor Conditions

<i>Parameter</i>	<i>Operating Condition</i>
Operating Temperature	150°C
Operating Pressure	15 atm
WHSV	1.0 hr ⁻¹
Catalyst Type	Amberlyst-36 resin
Catalyst Lifetime	2 years

After oligomerization, a hydrotreating step is used to saturate the remaining double bonds to finished paraffinic hydrocarbon fuels. In this step, the feed stream is mixed with fresh and recycled hydrogen from the process, and then heated to an inlet reactor operating temperature of 371°C and a pressure of 200 psig, [78]. As this is a relatively straightforward step for this pathway (hydrogenation), but is otherwise outside the scope of planned experimental work at NREL or ORNL, the model currently assumes similar design and cost details as the final hydrotreating step for the acids case, and a severity equivalent to a typical petroleum naphtha hydrotreater with a WHSV of 5 hr⁻¹ utilizing a 5% Pd/C catalyst [79-82]. A final distillation column fractionates the hydrocarbon products from the light gases, with the latter routed to the boiler.

Fermentation/Product Recovery: Acids

The production of carboxylic acids was identified in early 2015 as a potential strategy to anaerobically produce a biological intermediate that could be further upgraded to a hydrocarbon fuel via chemical catalytic conversion. Initial exploration focused on biological production of hexanoic acid via *Megasphaera elsdenii*, a natural lactic acid utilizing bacteria isolated from cow ruminant that has been shown to naturally produce acetic (C2), butyric (C4), valeric (C5), and hexanoic (C6) acids [79-83]. Given challenges associated with the conversion of xylose, the focus shifted to prospecting other potential hosts for improved production and conversion at the cost of acid chain length.

Subsequent downselection of C2–C4 producing anaerobic strains led to three strong candidates, *Clostridium butyricum* (ATCC 19398), *Clostridium tyrobutyricum* (ATCC 25755), and *Clostridium carboxidivorans* P7 (ATCC BAA-624), which all showed naturally high carbon diversion to acid products. However, a key challenge with this approach is the product toxicity at high titers which mandates pH control (adding large costs to the fermentation) or continuous removal of acids as they are produced [84-86]. Recent NREL R&D efforts have demonstrated the ability to produce acetic and butyric acids at high overall fermentation performance on both C5 and C6 sugars (i.e., high yields at 0.45 g/g sugars with nearly 100% overall utilization of major sugars and 1.1 g/L-hr productivity using *Clostridium butyricum* in batch fermentation) with concurrent production of hydrogen.

Biological acid toxicity/inhibition is a well-known phenomenon, and similar to ethanol or BDO toxicity the titer of the product species often determines the onset of cell inhibition. Differing from alcohols, an acid product has the added contribution of pH which can modulate the “apparent” titer of the toxic protonated acid form and affect the redox state of the host cell prompting metabolic shifts in certain cases [87]. Concurrent to the down-selection process a biological and a process strategy was pursued to overcome this toxicity barrier. Biologically, natural strains vary dramatically in their ability to tolerate titers and pH; therefore, the NREL R&D team pursued a campaign to identify genetically tractable, acid-tolerant organisms (with high tolerance to organic acids specifically), capable of a broad sugar utilization range and with high tolerance to biomass hydrolysates. While this effort is ongoing and has identified multiple strains of interest possessing several of the desired traits, to date no strains demonstrate all of the desired characteristics. Accordingly, efforts have focused on engineering several acid-tolerant yeast species for expanded sugar utilization capabilities and elevated tolerance to butyric acid in low pH environments.

From a process perspective, operating fermentations with *in situ* product removal minimizes accumulation of toxic products in the broth and hence avoids cell inhibition [88-93]. Furthermore, *in situ* product removal has no inherent upper limit on productivity/rate since the removal rate of acid products is a function of the extraction unit sizing, not an underlying enzymatic/physiological mechanism. Finally, operating at low extracellular product titers promotes higher secretion/excretion rates driving a stronger productivity throughout the fermentation. Despite the advantages *in situ* product removal systems provide, recovery of acetic acid—in particular across a pertractive membrane—has proven challenging to date, resulting in elevated carbon losses in cases that include this acid component.

Metabolic modeling work indicates a Fd-H₂ cofactor in *Clostridia* that is used to maintain redox balance when producing butyric acid [94, 95]. Presence of this cofactor provides a feasible metabolic engineering approach to eliminating acetic acid production, increasing hydrogen yield, and enabling better product recovery of butyric acid alone with an *in situ* system. As an added benefit, hydrogen

released during fermentation can be recovered and used in downstream catalytic reactions. For the current design, a recombinant *C. tyrobutyricum* strain engineered to anaerobically produce butyric acid as well as hydrogen from clean DMR hydrolysate is assumed, with the stoichiometries and conversions shown in Table 14.

Table 14. Acids Pathway Stoichiometry and Key Conversions

Reaction	Reactant	% Diverted to Reaction
Glucose + 0.018 DAP + 0.37 Nutrient → 6 <i>C. tyrobutyricum</i> + 2.4 H ₂ O	Glucose	5%
Glucose → 1 Butyric + 2 CO ₂ + 2 H ₂	Glucose	95%
Xylose + 0.015 DAP + 0.3087 Nutrient → 5 <i>C. tyrobutyricum</i> + 2 H ₂ O	Xylose	15%
6 Xylose → 5 Butyric + 10 CO ₂ + 10 H ₂	Xylose	85%
Arabinose + 0.015 DAP + 0.37 Nutrient → 5 <i>C. tyrobutyricum</i> + 2 H ₂ O	Arabinose	2%
6 Arabinose → 5 Butyric + 10 CO ₂ + 10 H ₂	Arabinose	85%
Sucrose + 0.036 DAP + 0.7404 Nutrient → 12 <i>C. tyrobutyricum</i> + 3.8 H ₂ O	Sucrose	5%
Sucrose → 1.9 Butyric + 4.4 CO ₂ + 5 H ₂	Sucrose	95%

^a CSL and DAP are both nitrogen sources required for growth. The stoichiometry shown above is only used to balance the compositions assumed for cell mass.

The biological conversion of sugars to butyric acid operates in fed batch using clarified and concentrated sugars exiting the continuous enzymatic hydrolysis system. Given the removal of solids upstream through CEH, the use of clarified sugars reduces membrane fouling and improves mixing hydrodynamics, which minimizes the occurrence of low pH or high titer pockets in the broth (leading to cell death/inhibition). The use of *in situ* acid removal across the pertraction membrane may theoretically allow for moving to continuous or semi-continuous modes of fermentation operation, which would improve capital utilization efficiency of the fermentation vessels. However, as membrane lifetimes, back-extraction of solvent, and other dynamic interactions with the fermentor broth over extended time periods are not yet well-understood, such extended fermentation modes are not presently assumed here. The assumptions for seed train design and conversions are maintained consistently with the details discussed in the 2011 ethanol report, including a 10% split of feed sugar substrate to inoculum growth, a five stage 10:1 volume increase per stage up to 200,000 gal (757 m³) prior to production reactor transfer, and two seed trains. This may be conservative for the present design utilizing concentrated hydrolysate with fewer production fermentor vessels and may be revisited in future design updates, potentially based on the use of the ACM models discussed above to provide a more realistic understanding of the dynamics of cell growth between the seed and production vessels and tradeoffs between feed sugar splits versus inoculum concentration in the production stage.

Fermentation occurs in large 1 MM-gal vessels and each production tank has a cooler to maintain temperature at a constant 37°C and an agitator to maintain cells in suspension. *In situ* product removal occurs continuously; as the fermentation progresses acid product is removed using a liquid-liquid membrane extraction system (membrane pertraction) connected through a pump-around loop. Targeted productivity remains high throughout the fermentation at 2.0 g/L-hr acid production (based on targets set by NREL researchers), requiring 3 fermentor vessels. Relative to the ethanol design case (and the basis maintained for BDO fermentation) which minimized agitation power to keep the broth in suspension, this design triples the agitator power demand from 0.15 to 0.45 hp per 1,000 gal (88.6 KW/MM L), given stronger organism sensitivity to product (acid) titer in the broth and thus a need to maintain better homogeneity as the broth circulates through the membrane. Alternatively, or perhaps in addition to this adjustment, a smaller vessel size may plausibly also be required for the same reason,

but this is not yet well understood until more detailed design/operational parameters are established for the acids fermentation/membrane pertraction system.

The process assumes complete consumption of glucose, xylose, arabinose, and sucrose, of which smaller fractions are converted to the acids products as shown in Table 14, resulting in an overall process fermentation yield of 0.433 g butyric/g sugar, equivalent to 89% of the maximum theoretical metabolic yield. The key carboxylate fermentation metrics are listed in Table 15 below.

Table 15. Key Butyric Acid Fermentation Parameters

Organism	<i>Clostridium tyrobutyricum</i>
Temperature	37°C (99°F)
Productivity	2.0 g/L-hr
Fermentation vessel volume	3,785 m ³ (1 MM gal)
Fermentation vessel agitator power demand	0.45 hp/1,000 gal (88.6 KW/MM L)
Corn steep liquor seed requirement	1.3 (g/g feed)
Corn steep liquor production requirement	0.66 (g/g feed)
Diammonium phosphate seed requirement	8g/L fermentation broth
Diammonium phosphate production requirement	0.495 g/L fermentation broth
Inoculum production: number of seed trains	2
Inoculum production: number of batch stages	5
Inoculum production: maximum stage volume	200,000 gal (757 m ³)
Fermentation process yield (g butyric/g sugar)	0.433

The pertractive *in situ* product removal system relies on a tri-octyl-phosphine oxide (TOPO)-assisted organic phase to selectively remove acid from the broth across a membrane [96, 97]. Short to medium chain acids show relatively low partitioning to the organic phase due to their significant polarity. To overcome this poor separation, TOPO, which is a strong hydrogen bond acceptor with poor water solubility, is added to the organic phase. The addition of TOPO causes complexation with the protonated acid species and functions as a “carrier” molecule increasing the recovery for shorter acid species. Because complexation is tied to the protonated species exclusively, the efficacy is governed by a multispecies pH-dependent equilibria with effectiveness a function of pKa (i.e., chain length) and process pH (i.e., strain pH toxicity) as shown in Figure 10 [98].

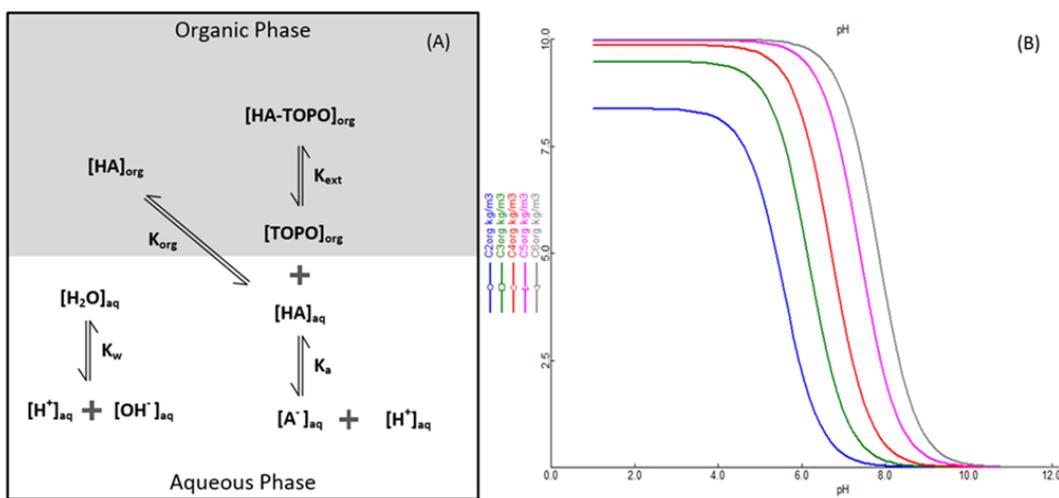


Figure 10. Acid extraction equilibrium and predicted recovery in unit

The design case uses a liquid-liquid membrane contactor, wherein an aqueous broth phase is fed through the shell side and put in contact with hydrophobic polymer membrane fibers carrying a mineral oil + TOPO organic phase on the tube side. A mild shell-side pressure maintains intimate contact relying on hydrophobic forces to prevent aqueous breakthrough to the organic tube side. The flow rate of the organic phase can be tuned to control the rate of product removal as needed based on the fermentation productivity, as well as target a specific broth acid titer/pH. In the current design, *C. tyrobutyricum* is assumed to tolerate a pH of 4.7-5 in the broth, conditions at which the modeled extraction equilibrium predicts a recovery of 100% of the butyric acid in the aqueous phase (but as noted previously a lower recovery of any acetic acid).

After extraction to the organic phase, a vacuum is pulled on the mixture and it is routed to distillation for acid purification. The vacuum distillation is critical to prevent dimerization and degradation of the TOPO carrier molecule as well as reduce the boiling point improving the energy efficiency of the integrated plant. The acid is recovered in high purity from the distillate while the mineral oil and TOPO exits from the bottom and is recycled back to a storage tank for reuse in the pertractive unit. Table 16 lists the key pertraction metrics and design assumptions.

Table 16. Petraction Operating Specifications

<i>Parameter</i>	<i>Operating Condition</i>
Membrane type	Hydrophobic
Operating temperature	Ambient
Operating pH	4.7
Transmembrane pressure	~15 psig
Solvent	Mineral oil
Butyric acid recovery	100%

Catalytic Upgrading: Acids

The recovered butyric acid exiting the column is re-pressurized to atmospheric pressure then routed to the catalytic upgrading process. This three-step conversion process consists first of acid condensation/ketonization, followed by ketone condensation to higher molecular weight enones, and finally upgrading of enone intermediates to drop-in hydrocarbon fuels [99]. The additional condensation step allows the pathway to target diesel- and jet-fuel range branched hydrocarbons with a blendstock in the 14-carbon chain length range. The conversion steps are illustrated in Figure 11 with further details provided below.

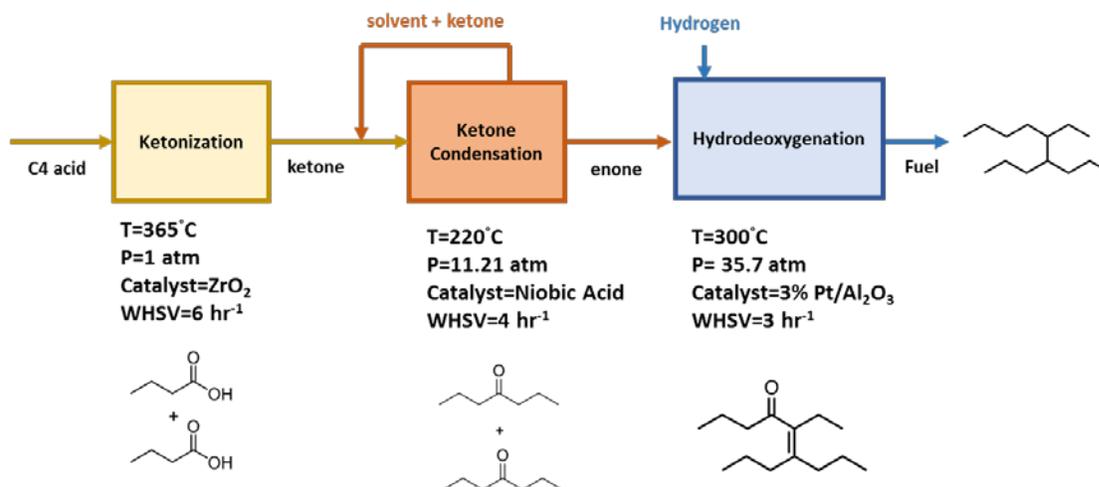


Figure 11. Acid upgrading reaction steps with key metrics

The first step of the process converts the butyric acid to a range of ketones under ambient pressures and elevated temperature (365°C) [100]. The upstream distillation yields nearly pure butyric acid, which is completely converted to 4-heptanone over an acidic ZrO₂ catalyst. The condensation releases one mol of carbon dioxide per two mols butyric acid resulting in a net yield of 0.65 g 4-heptanone/g butyric acid feed and proceeds rapidly with a WHSV of 6 hr⁻¹ and a 2-year catalyst lifetime. Heat integration between the effluent and feed reduces the energy demand and a hot oil heating system served by a direct fired heater is used to achieve the high-temperature feed setpoint.

After ketone condensation the product stream is cooled to 50°C then flashed to separate the CO₂ from the liquid phase with roughly 17% of the 4-heptanone volatilized to the vapor phase during the flash. The 4-heptanone lost in the vapor stream exiting the flash is ultimately recovered via a water scrubber followed by a decanter for phase separation. This recovered 4-heptanone is then recombined with the flash liquid stream resulting in an overall 96.5% recovery of the acid condensation intermediate for further upgrading. Table 17 shows the key specifications for the initial ketonization reaction.

Table 17. Ketonization Reaction Parameters

<i>Parameter</i>	<i>Operating Condition</i>
Acids-to-Ketones (wt% acids)	100%
Operating Temperature	365°C
Operating Pressure	1 atm
WHSV	6.0 hr ⁻¹
Catalyst Type	ZrO ₂
Catalyst Lifetime	2 yr
Overall Ketone Recovery (wt%)	96.5%

To produce a diesel- and jet-fuel range blendstock with improved cold flow properties, the seven carbon ketone intermediate is further upgraded via condensation which promotes branching and extends the hydrocarbon to a C14-length enone [101, 102]. Since 4-heptanone is a less reactive central ketone component, to boost the single-pass conversion through condensation the conversion step requires the addition of a heterogeneous catalyst (niobic acid) and a solvent to mitigate catalyst

inhibition over a longer 15-hour residence time in a stirred tank slurry reactor. In the current design, the liquid feed is pressurized to 150 psig and mixed with toluene to achieve a 3.7:1 solvent-to-ketone ratio (w/w). Toluene displays beneficial solvent properties associated with the stable aromatic structure which prevents and minimizes solvent cracking to light hydrocarbons at the reaction conditions compared to a similar linear alkane equivalent. Catalyst is added in sufficient quantity to achieve a 1:4 catalyst-to-ketone ratio by weight and the system is heated to 180°C. The reaction proceeds slowly in a CSTR sized to achieve a mean residence time of 15 hours. At these conditions, the single-pass conversion is 60% with 100% conversion to the C14 enone. The reaction produces 1 mol of water per mole of enone, which phase separates cleanly along with the solid catalyst and is filtered to remove the aqueous solution then recycled for reuse. The enone, toluene, and unreacted ketone are then distilled, separating the lighter boiling toluene solvent and ketone as distillate, which is recycled back to the reactor feed and mixed with the pure acid condensation feed until extinction. The heavy C14 enone exits the column bottoms along with minor amounts of the 4-heptanone at a temperature of 344°C. To reduce energy use and heat demands, the distillation is performed at a lower 73 psig, though even at reduced pressures the high boiling point enone mandates use of the hot oil system for the reboiler. Table 18 lists the key operating specifications for the ketone condensation step.

Table 18. Ketone Condensation Reaction Parameters

<i>Parameter</i>	<i>Operating Condition</i>
Ketones-to-Enones Conversion (% ketones feed)	60%
Operating Temperature	180°C
Operating Pressure	150 psig
Catalyst: Ketone Loading (w/w)	0.25
Solvent: Ketone Loading (w/w)	3.65
WHSV	15 hr CSTR
Catalyst Type	niobic acid
Catalyst Lifetime	2 years

Following ketone condensation, the product enters a fuel finishing step, where the enone intermediate (and any unconverted ketone and solvent intermediates) are fully deoxygenated over a 3% Pt/Al₂O₃ catalyst in the presence of hydrogen at a pressure of 35 atm. Makeup hydrogen is fed to achieve a 24.6:1 molar ratio to the oxygenated feed entering the reactor. The reactor achieves complete hydrogenation to saturated hydrocarbon products operating at a WHSV of 3 hr⁻¹. The product stream is cooled, and excess hydrogen is recovered in a cold high-pressure separator, then recompressed and recycled to the hydroprocessing unit. The C14 branched diesel blendstock is recovered then sent to storage. As noted previously, hydrogen produced during the fermentation is separated from the other vent vapors via pressure swing adsorption and fed to the hydrotreater. In the current design the butyric acid fermentation provides a surplus of hydrogen and no supplemental makeup hydrogen is required for upgrading. Table 19 shows the key specifications for the fuel finishing reaction.

Table 19. Fuel Finishing (Hydrotreating) Reaction Parameters

<i>Parameter</i>	<i>Operating Condition</i>
Hydrotreating (HDO) (%)	100%
Operating Temperature	270°C
Operating Pressure	35 atm (500 psig)
Hydrogen: Feed Loading (molar)	24.6
WHSV	3 hr ⁻¹
Catalyst Type	3% Pt/Al ₂ O ₃
Catalyst Lifetime	3 yrs

3.5.3 Cost Estimation

For the BDO case, fermentation takes place in the same physical vessels as hydrolysis (sequential hydrolysis and fermentation, similar to the 2011 ethanol case)—utilizing the 1 MM-gal batch stirred tank bioreactors. However, for cost allocation purposes, the fraction of total batch time and associated volume spent in fermentation is allocated to Area 500 and vice-versa for hydrolysis allocated to Area 300. All design/cost details for the main fermentation and seed equipment are described in the 2011 ethanol design report; briefly, the large 1MM-gal fermentors, fourth and fifth seed fermentors (including cooling coils), and seed hold tank were quoted by Mueller Co. The smaller first, second, and third seed fermentors were quoted by A&B Process Systems Corp. and are skidded units with jacketed cooling and agitation included. The lignin press following fermentation is based on the same unit as originally quoted in the 2011 ethanol report, as utilized for lignin dewatering from beer column stillage.

A filtered hydrolysate storage tank with a residence time of 20 minutes is included to provide intermediate storage for filtrate from the belt filter. The clarified BDO polishing filtration system includes two parallel skid microfiltration units, including clean-in-place (CIP) system and backwash. Installed equipment cost is \$1.6 MM total for the two skids. The ion exchange system uses a separate-bed configuration, with strong acid cation and weak base anion resins. Estimated installed equipment cost is \$4.5 MM including the resins, based on scaling from cost quotations provided by Harris Group in NREL's 2015 design case (the provided cost did not break out equipment versus resin cost details separately). In total, installed capital costs for the solid separation and polishing steps are estimated at \$12.1 MM. The BDO upgrading and oligomerization reactors were both costed based on the APR reactor in the NREL 2015 catalytic upgrading design case [9], with costs scaled based on the full flow rate into the reactors. Costs for hydrotreating (hydrogenation) were set consistently with the hydrotreater utilized in the acids case (discussed below), after adjusting for more mild operating conditions in this case. All catalyst costs are summarized in Section 4.3.

Although the 2,3-BDO upgrading reactor exhibits the ability to process a high level of water, more concentrated BDO levels with less water would reduce reactor capital costs as well as heat demand to raise the temperature of the feed stream from 35°C to 250°C. Compared with conventional distillation, membrane pervaporation may be an alternative option with a lower energy demand. For example, ORNL is investigating a “HiPAS” membrane system that may offer a more energy efficient, larger flux, and economical separation option for BDO concentration. Without operating/design details for this system, on a high level, the installed capital cost for this addition would need to be below \$17 MM to offer net MFSP savings through lower energy demands if 50% of the water could be removed through this operation.

In general for the acids case, the acid fermentation units maintained the same equipment and cost basis as the BDO case (based on the 2011 ethanol design report). Fermentation vessels continue the use of 304SS to accommodate corrosive environments more pronounced with the production of carboxylic acids. The same seed train equipment/costs are also maintained consistently with the BDO case, based on the 2011 report. The pertractive membrane extractor system is based on a vendor cost estimate as well as guidance and costing for vacuum distillation for solvent recovery. The acid condensation reactor maintains a similar basis as the catalytic APR reactor design described in the 2015 catalytic design report [9].

The recovery flash, scrubber tower, and decanter costs were estimated using Aspen Capital Cost Estimator (ACCE) along with the process stream phase separation properties [103]. The ketone condensation reactors and catalyst filtration unit and solvent recycle tower were costed using ACCE. The reactors are modeled as continuous stirred tank units and account for the residence time at the modeled flow rate. The hydrodeoxygenation reactor is designed as a fixed bed hydrotreater with hydrogen mixing internals. The base reactor price quote was estimated based on prior NREL TEA studies on hydrotreater equipment capital costs and correlations to liquid feed volume flow. The base conditions for the hydrotreater (pressures >1000 psig and temperatures >310°C) were de-escalated to the current 500 psig operating pressure using the Guthrie pressure factor approach and the reactor size was scaled according to the total liquid volume feed entering the reactor. The hydrogen makeup compressor is a five-stage reciprocating unit, and the recycle compressor is designed as a centrifugal compressor due to the lower pressure increase in the recycle loop. Both compressor estimates include a spare unit.

3.5.4 Achieving the Design Case

For the BDO pathway, despite the relatively recent R&D focus at NREL on this strategy, all key fermentation parameters have already been demonstrated within 10%–15% of their future targets, namely BDO process yield (0.42 g/g versus targets of 0.47 g/g), sugar consumption (approaching final targets for overall glucose and xylose utilization), and BDO productivity (1.7 versus 2.6 g/L-hr). Arabinose utilization remains low to date (less than 10% converted to BDO) but this carries a much smaller cost impact than glucose and xylose, although high unconverted arabinose may increase risk for contamination and will be targeted for improvement. Similarly, performance benchmarks observed at ORNL for the BDO upgrading steps have also been demonstrated to be working well, leaving high confidence in the ability to achieve final targets by 2030. However, the largest technical hurdle that remains for this pathway is in engineering the *Z. mobilis* organism to eliminate the dependency on (minimal) oxygen demands for cell redox balancing, thereby making the fermentation fully anaerobic. Unlike the ethanol pathway, BDO production generates a surplus of NADH, which must be oxidized to balance cellular redox. In the presence of oxygen, the organism can oxidize NADH to NAD⁺ using the native NADH dehydrogenase. Current experimental efforts at NREL are working on improving the redox balance by developing strategies to eliminate oxygen requirements by redirecting metabolic flux to convert excess NADH through H₂ generation or introducing the NADH requiring succinate pathway (thus yielding either hydrogen or succinic acid coproducts). The former is assumed in this work.

In the event such BDO strain engineering efforts are unsuccessful, the onus would fall on the TEA modeling efforts to better understand reactor design, operation, and cost implications for microaerophilic bioreactors, which are currently a less explored space than fully anaerobic or fully aerobic fermentation. For example, recent consultation with industry has established that if low

dissolved oxygen (DO) levels must be maintained within a strict window, this may incur similar costs and challenges as more fully aerobic fermentation (where DO uniformity would be improved by moving to smaller vessel sizes but also may be improved through increased agitation or pressure control), thus losing the advantages of anaerobic fermentation versus aerobic as described above. Initially, this was a concern for this pathway, as too little oxygen favored production of ethanol and too much favored production of a byproduct, acetoin. However, more recently ethanol coproduction has been knocked out entirely, and fermentation optimization activities have demonstrated the ability to minimize acetoin (and furthermore, catalytic upgrading activities have also demonstrated the ability to upgrade acetoin with equal performance and yields as 2,3-BDO, making any co-production of acetoin less problematic). For this reason, recent state of technology models reflecting current fermentation benchmarks have asserted the use of similar 1 MM-gal CSTR vessels as are utilized for fully anaerobic fermentation, but merely with air intake vents to allow for the presence of air/oxygen in the fermentor headspace. When coupled with potentially higher agitation mixing, this scenario is envisioned to provide sufficient DO levels in the bulk fermentation broth, even if not homogeneous throughout the full fermentor volume; this concept has been experimentally demonstrated to provide similar fermentation performance using air overlays in the fermentor headspace as air sparging into the bottom of the fermentors, albeit limited to bench-scale fermentation volumes. Moving forward, computational fluid dynamics (CFD) modeling may help to understand optimal microaerophilic bioreactor design and operation, by quantifying tradeoffs between fermentor size versus agitation power demands to provide satisfactory bulk DO concentrations.

For the acids pathway, while the majority of all key fermentation parameters have similarly been shown to be performing well relative to future targets (i.e., productivity of 1.1 g/L-hr versus 2.0 g/L-hr targets with process yields nearly at target levels), one of the largest uncertainties in the current design is the continuous separation strategy to recover the acid from the fermentation broth via pertractive membranes. Such operations could suffer from a number of potential processing failures including toxicity due to failure to control the pH from inefficient acid removal, potential fermentation contamination due to solvent back-filtration across the membrane into the fermentor broth, or plugging of membrane filters, to name a few. To date, acid recovery has been demonstrated to be high over short-term trials using clean substrates (including nearly 100% recovery of butyric acid specifically), but encounters more challenges using real hydrolysate substrate broth. Over a longer timeframe, the continuous recovery and recycle of the solvents may encounter challenges if other acids or molecules extract and build up in the solvent loop, which would require periodic replacement of one or both solvents. Longer-term implications on membrane lifetimes, fouling, pump-around throughput rates, etc. are not known at this time, and will require further study in the future as more granular operational and design details are established for this system. While pH-controlled fermentation to maintain acids as salt complexes at elevated pH (followed by ion exchange and neutralization) can be shown to work well experimentally, the associated costs for acid and base addition, as well as subsequent salt disposal, would be untenable.

A potential mitigation strategy is being explored in the DOE BETO-funded Bioenergy Separations Consortium. For this approach, the fermentation is controlled at a neutral pH via the introduction of a caustic solution and the separation strategy uses a resin wafer based electrodeionization operation that separates the conjugated base. The operation targets a nearly complete recovery and separation of the acid and base. The carboxylic acid product is sent on for further upgrading as outlined in the above design. The base is recycled to the fermentation reactor, limiting any caustic make-up requirement. The key factors that will make such an operation economically viable and align with sustainability

goals of the integrated biorefinery hinge not only on high recovery of both the acid and the base but also the reduction of electricity demand. Recent work by Argonne National Laboratory under the Bioenergy Separations Consortium has demonstrated the reduction of both capital cost and electricity demand compared to many documented electro dialysis systems[104, 105].

Acid upgrading work has demonstrated the complete three-step conversion to a final fuel product (including initial fuel testing data), although these results have not been tested on acid extracted DMR fermentation broth and remain unoptimized in that regard. While there are additional challenges associated with an extracted catalytic acid feedstock compared to a pure substrate (e.g., minor broth impurities and entrained water), discussions with researchers point to clear mechanisms for attenuating these effects. The acid condensation reaction catalyst can be broadly tuned for acidity and is expected to tolerate up to 10% water; furthermore, because the catalyst lacks exotic metal atoms, poisoning is not expected to be an issue. After the initial catalytic step, the scrubber and phase separation of the intermediate separation scheme will preclude further downstream issues associated with impurities. Using clean butyric acid, current demonstrated yields for the acid condensation step are near 100% with very high selectivity in excess of 90% to the desired 4-heptanone product. Ketone condensation proceeds with high selectivity to the desired enone product under the controlled lower temperature conditions with toluene as a solvent, with the current focus on reducing the residence time to the 15-hour target or less.

Current work is also exploring a solventless “neat” configuration (i.e., greatly reduced capital costs) but suffers from low conversion and poor selectivity to the desired fuel molecule to date. Similarly, a high-temperature approach achieving near complete conversion is being explored but causes excessive condensation to heavier less desirable fuel products. The final hydrotreating step is generally considered established technology and not currently a focus of NREL R&D. In the future, as upstream conversions improve, renewed focus on HDO may find further improvements or updated targets that improve the overall economics, such as platinum loading or WHSV.

3.6 Area 600: Wastewater Treatment

3.6.1 Overview

Wastewater is generated in the process from condensed pretreatment flash vapor in Area 200, the fermentation broths in Area 500 and 700 (after separation of product and cells), and minor sources such as boiler and cooling tower blowdown. All such wastewater is sent to the WWT system in Area 600. After treatment, the effluent water is assumed clean and fully reusable by the process, reducing both the fresh makeup water requirement and discharge to the environment.

In previous design reports, the chemical oxygen demand (COD) loading to wastewater treatment was relatively large due to high concentrations of soluble unconverted biomass components, primarily extractives. These components ultimately arrived at WWT in the stillage or aqueous phase post-fermentation, or in the black liquor produced in deacetylation. NREL consulted with Brown and Caldwell in 2010 and again in 2012 to design treatment schemes that included anaerobic digestion of 80% of this organic material to biogas, followed by aerobic digestion of the remaining organics and final cleanup by reverse osmosis. The biogas was used as boiler fuel for heat and power, and the reverse osmosis (RO)-treated water was recycled to the process.

In the present design, the black liquor containing the extractives as well as soluble lignin is combined with further deconstructed solid lignin and sent to aerobic fermentation with *Pseudomonas putida* in Area 700. Given the scavenging nature of *P. putida*, we reasoned that these extractives components would likely be consumed in the aerobic fermentation, forming cell mass and CO₂ as well as some organic acids, as dictated by the organism’s engineered metabolism (discussed in the next section). Given the elimination of extractives, and drastic reduction in other organics solubilized to DMR black liquor (i.e., carbohydrates and solubilized lignin) that ultimately reach WWT given the addition of the Area 700 train, COD loading in the WWT feed stream is reduced by about 92% (acids case) and 82% (BDO case, given lower overall sugar utilizations) relative to the 2013 design report (9 and 21 g/L respectively versus 120 g/L in the 2013 design), obviating the anaerobic digestion requirement. The present design therefore begins at aerobic digestion; the updated simplified flow diagram is shown in Figure 12.

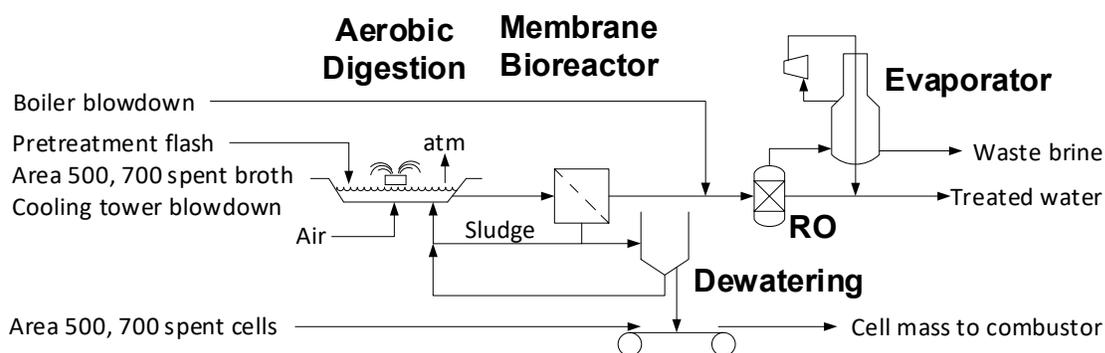


Figure 12. Simplified flow diagram of the WWT process

The aerobic system comprises several large basins or ponds that are aerated from the bottom via a grid sparger. The water in the basins is continuously cycled through membrane bioreactors, which are aeration tanks with ultrafiltration membranes that yield a clean water stream and a low-solids biomass sludge stream, which is mostly recycled to the basin. The wasted fraction of sludge that is not recycled passes first through a gravity belt thickener, then is subsequently centrifuged to >20% solids. The fermentation cell mass separated in Areas 500 and 700 is collected along with the digester sludge, and the combined solid mass is routed to the boiler. The water effluent of the membrane system is sufficiently clean to feed directly to RO to remove dissolved salts. The RO permeate is recycled to the process and the RO retentate is concentrated in an evaporator to produce a brine, sold in this design as a co-product.

3.6.2 Design Basis

The present WWT system follows the design basis from the 2012 Brown and Caldwell subcontract, as detailed in the 2013 design report, from aerobic digestion forward. In the Brown and Caldwell design, the anaerobic system removed 80% of the influent COD, transferring 2.67 MM gal/d of water to aerobic treatment at 13.3 g/L COD. For the acids case, the hydraulic load to aerobic treatment is larger than this, but COD loading is lower. For the BDO case, the hydraulic load is smaller but COD load higher. Nitrogen loading in both cases is significantly lower than assumed in the Brown and Caldwell design—this indicates that supplemental ammonia will be required to support culture growth. The relevant design parameters of the wastewater system are summarized in Table 20.

Table 20. WWT System Design Basis

Aerobic digestion influent conditions	2012 Brown and Caldwell design (used for scaling)	This design (acids case)	This design (BDO case)
Hydraulic load	2.7 MM gal/d	2.8 MM gal/d	2.2 MM gal/d
Total COD	13.3 g/L	9.3 g/L	21 g/L
Total Kjeldahl N	724 mg/L	66 mg/L	38 mg/L

The wastewater feed is pumped to the aerobic activated-sludge basin. The basin construction is concrete and steel. Air is delivered through a submerged grid sparger; surface aerators are also specified to enhance evaporative cooling during summer months. In aerobic digestion, 96% of the soluble organic matter is removed, with 74% producing water and carbon dioxide and 22% forming cell mass. The contents of the pond are cycled continuously through membrane bioreactors for clarification.

The membrane retentate is a low-solids sludge stream that is mostly recycled back to the basin. A fraction of the sludge is removed from the loop and pumped to a dewatering system. Brown and Caldwell specified gravity belt thickeners to first concentrate the sludge to 4% solids, followed by centrifuges with 95% solids capture rate and a cake concentration of 20% solids. The centrate is recycled with polymer addition to the aerobic basins. Dewatered sludge is then conveyed to the combustor in A800. The treated water is pumped to a RO membrane system for salt removal. RO produces a brine containing primarily sodium sulfate along with all remaining ions and organics. The brine is further concentrated in a mechanical-vapor-recompression evaporator to 50% solids and the condensate is also recycled to the process. Finally, the brine is further processed through a dryer and centrifuge to crystallize the salt for sale as a coproduct. This was deemed necessary in the present model configuration in light of the substantial quantities of caustic (sodium hydroxide) and sulfuric acid used in multiple points throughout the facility, which would incur unreasonable costs without either recovering those input chemicals or else offsetting a portion of the chemical costs by selling the sodium sulfate salt. The latter is elected here given that the salt is already produced at high purity as a byproduct from wastewater treatment (over 98% purity of the brine solids).

3.6.3 Cost Estimation

Brown and Caldwell estimated the capital costs of the wastewater system components, drawing on support from technology vendors. In previous design reports, the individual unit costs were scaled to either the hydraulic flow rate or COD load to anaerobic digestion. For the present model, with anaerobic digestion removed, the remaining components (aerobic digestion, sludge dewatering, reverse osmosis, evaporation, and centrifugation) were re-baselined to the total flow and COD loading of the stream leaving anaerobic digestion in Brown and Caldwell's design (2.67 MM gal/d at 13.3 g/L COD) and scaled from there. Additional equipment costs for sodium sulfate purification were scaled from a recent subcontract with Nexant for an evaporation flash drum, dryer, and centrifuge designed for this purpose.

Table 21. Installed Capital Costs for Area 600

Equipment	Acids case	BDO case
Aeration basins	\$9.5 MM	\$8.1 MM
Membrane bioreactor	\$7.8 MM	\$6.0 MM
Reverse osmosis system	\$4.2 MM	\$3.2 MM
Dewatering	\$2.4 MM	\$3.3 MM
Others (pumps, conveyer, etc.)	\$3.5 MM	\$4.8 MM
Brine evaporator	\$7.7 MM	\$6.6 MM
Sodium sulfate purification	\$3.9 MM	\$3.6 MM
Totals	\$38.8 MM	\$35.6 MM

3.7 Area 700: Lignin Upgrading

3.7.1 Overview

This process area covers the key unit operations for deconstruction and conversion of lignin (and other residual biomass components) to coproducts, as a critical element to enabling the \$2.50/GGE MFSP targets for biochemical processing. In summary, the black liquor product from DMR pretreatment is combined with the residual solids stream separated during CEH (acids case) or from fermentor broth clarification (BDO case) and routed to a more severe “base catalyzed deconstruction” (BCD) unit employing a caustic soaking process at elevated temperature to further deconstruct high-molecular weight lignin to metabolically accessible compounds. The caustic from DMR pretreatment that exits with the black liquor offsets a large portion of the caustic required to achieve the elevated pH in the BCD step. The soluble liquid BCD product is then routed to bioconversion, which converts soluble lignin and other residual organics to muconic acid through an aerobic pH-controlled bioconversion with *P. putida*. The product is initially produced as a muconate salt at the given fermentation pH (i.e. the caustic from DMR/BCD neutralizes muconic acid to maintain near-neutral pH forming sodium muconate), which is then isolated in high purity as muconic acid crystals following acid addition and low-pH crystallization. The muconic acid crystal is redissolved in a carrier solvent then hydrogenated under mild conditions to adipic acid, which is subsequently recovered through another crystallizer. A schematic diagram for the process is shown in Figure 13.

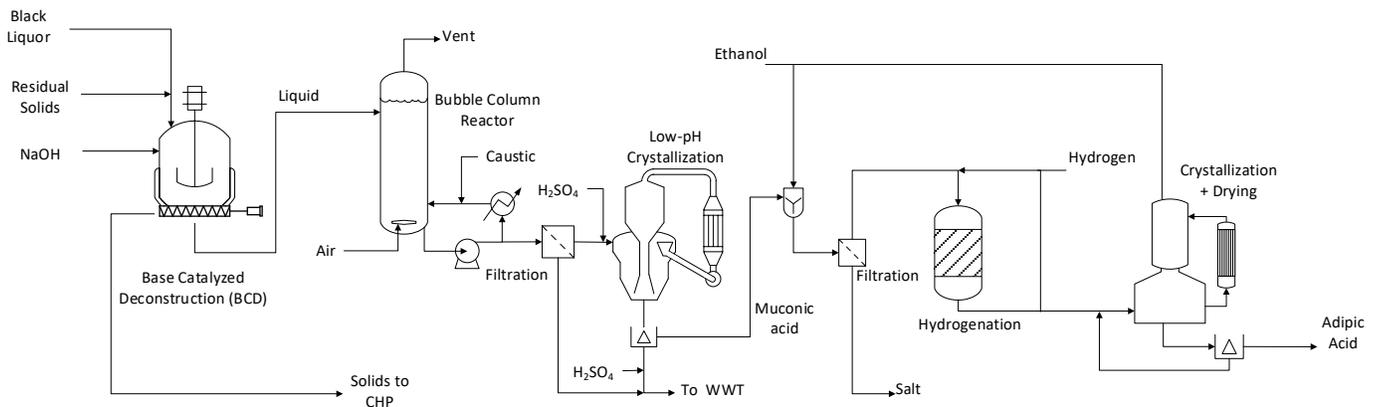


Figure 13. Schematic diagram of lignin deconstruction and conversion process to coproducts

Historically, in prior biochemical designs residual lignin and solids were burned using a high-solids biomass boiler to produce steam and power for the process, which realizes minimal additional economic value to the carbon present in the lignin but does offset power and natural gas (NG) imports which substantially improve the sustainability of the integrated process design. A second option is to upgrade a fraction of the available lignin/unconverted carbon to a value-added coproduct. The 2013 biochemical design report presented an initial analysis around lignin utilization to coproducts, ultimately concluding that nonoxygenated lignin coproducts (e.g., cyclohexane) provide limited opportunity for achieving \$3/GGE or lower cost targets, as well as showed an increase in overall greenhouse gas emissions when compared to the baseline design of burning lignin for heat and power. Other product options with higher atom efficiencies that produced oxygenated value-added chemicals were predicted to be viable for meeting such MFSP targets and improved overall sustainability of the integrated design, even when requiring power and natural gas imports.

In light of these early conclusions, research shifted to production of oxygenated intermediates that take advantage of the underlying structure of the biomass composition. While a wide array of coproducts are possible from lignin [106, 107], in this design, adipic acid is highlighted as a representative example coproduct from lignin. Adipic acid is an oxygenated di-carboxylic acid coproduct primarily utilized to produce nylon and other polymeric materials [11]. Not only is the market value of adipic acid ideal for meeting out-year \$2.50/GGE cost goals at roughly \$0.86/lb, but the direct replacement of adipic acid via the chosen process improves sustainability compared to traditional petroleum-derived adipic acid produced in a two-stage process that involves energy-intensive oxidation of cyclohexane followed by nitric acid oxidation of the intermediate to adipic acid [10]. The harsh latter steps of the synthesis have a large impact on the sustainability of the fossil-based process, which are absent in the current biological route [108]. Additionally, adipic acid possesses a large market volume over 2.3 MM tonne per year globally [11] (roughly 2.8 MM tonne/year currently), thus exceeding smaller “niche” market products that may enable high values but not at volumes that could sustain multiple biorefineries at commodity scale.

Valorization of residual carbon in the lignin rich solids requires three conceptual steps: deconstruction, conversion, and upgrading. During deconstruction, recalcitrant solids are subjected to chemical treatment to produce a more tractable material for subsequent conversion. During this step, the goal is to reduce the molecular weight of the substrate to promote solubilization and increase the amount of accessible chemical compounds entering the conversion stage. Alkaline pretreatment using a strong base increases the lignin solubilization owing to the deprotonation of the hydroxyl moieties of the macromolecule, and initiates cleavage of beta-O-4 bonds generating more accessible lignin monomers, dimers, and oligomers.

After deconstruction, the material is sent to the conversion phase, wherein the accessible carbon is fermented to a single desired product intermediate. Compared to catalytic approaches operating on complex mixtures that suffer from poor selectivity to any single product but high conversion of all substrates (e.g., pyrolysis oils and hydrothermal liquefaction), using a biological approach provides the opportunity for high selectivity to a single product and combines what otherwise requires multiple successive reaction and fractionation units. This high specificity is critical as many coproduct chemicals require high homogeneity and purity (particularly for products in technical markets such as polymers or nutritional supplements).

To achieve these desired outcomes and channel a diverse mixture of carbon compounds to a single desired product requires a strain capable of two major behaviors. First, a robust and diverse set of catabolic pathways covering acids, sugars, and aromatics is necessary for high conversion. Second, the ability to engineer a heterologous pathway or pathway(s) connecting the consumed substrates to a single product is necessary for high selectivity to a single product. Both of these phenomena are readily accomplished in isolation (e.g., mixed cultures often can exhibit high conversion of complex mixtures; highly engineered single strains show high selectivity to products from individual substrates). However, combining the two behaviors is challenging due to the frequently competing goals of the host regulatory network in catabolic strains and the lack of catabolic diversity in standard engineered hosts that do possess selective pathways. More recent work focused on expanding the industrially relevant host strains past the familiar *E. coli* and *S. cerevisiae* has enabled the rapid onboarding of a more optimal funneling host, *P. putida*. This host displays both desired behaviors, and importantly has proven to be genetically tractable to metabolic engineering strategies.

The final step following conversion is recovery and upgrading to the desired coproduct. Recent work has shown the successful use of temperature and pH to crystallize dicarboxylic acids (i.e., muconic acid and its downstream derivative adipic acid) from aqueous solution using the differing temperature solubility curves of the protonated/deprotonated species.

3.7.2 Design Basis

The lignin utilization process was designed based on existing literature, ongoing NREL research, and communications with select contractors in the field. Black liquor exiting the counter-current deacetylation reactor is combined with the residual solids exiting enzymatic hydrolysis (lignin press on the whole slurry material in the BDO case, and on the residual solids stream exiting CEH in the acids case). The residual solids consisting of ~70% lignin by weight enters at near ambient temperature as a ~40% solid paste/slurry.

As noted earlier in the report, the black liquor contains acetate, extractives, sucrose, carbohydrates, and nearly half of the original lignin present in the biomass (of which 15% is already in monomer form) as a low pH aqueous solution. This black liquor solution is routed directly from the reactor at 90°C and mixed with the downstream residual solids slurry, which reduces heating requirements for the subsequent deconstruction step. Combined, this mixture contains 99% of the lignin originally present in the biomass as a complex slurry of solids, solubilized solids, and soluble components. Table 22 shows the composition of the two feed streams.

Table 22. Composition of Both Lignin Streams in Model

<i>Parameter</i>	<i>Black Liquor</i>	<i>Residual Solids</i>
Total Solids ^a (wt %)	12.5%	63.1%
<i>Species Distribution (% total solids)</i>		
Lignin	52.9%	48.7%
Cellulose	5.0%	7.4%
Xylan	13.9%	1.2%
Arabinan	5.1%	0.1%
Other Solids (ash, protein, etc.)	23.1%	42.6%

^a Total solids defined as lignin, soluble lignin, cellulose, xylan, arabinan, manan, galactan, ash, and protein.

The combined stream is routed to a BCD reactor operating at elevated temperatures to further deconstruct the lignin and solubilized oligomers. Caustic is added to achieve a minimum of 2 wt% loading based on the feed mixture. In the current design, due to the higher caustic loading and more concentrated black liquor accompanying the counter current configuration, the combined mixture has a caustic loading of 5.1%, in excess of the 2% threshold and no additional caustic is needed. The treated mixture is pressurized to 6.3 atm to prevent vaporization throughout the duration of the reaction, then reacted for 30 minutes at a temperature of 120-160°C. At present the model assumes a basis of 120 °C based on latest experimental conditions, but research is ongoing to identify the most optimal temperature for this operation, and may be increased to as high as 160 °C if this is found to promote better solubilization/deconstruction to usable components. This step represents a key cost driver to the overall process, as evidenced in the “metabolically accessible lignin” parameter in the Sensitivity Analysis below (Section 5.2), and will require continued R&D focus to better understand and optimize moving forward.

Based on experimental work done at NREL, the more severe temperatures promote higher solubilization of the lignin solids, although there is a balance as increased severity eventually degrades the solids to a mixture of short chain acids and alcohol products. In the current design, 36 wt% of the solids entering the BCD reactor are solubilized to metabolically accessible monomers/oligomers. Of the solids present, this includes 48 wt% solubilization of carbohydrates and 53 wt% of the lignin. The mixture stream from this step is fractionated with the residual solids sent to the boiler, while the solubilized product is cooled and then routed to biological funneling. Table 23 summarizes the BCD reaction conditions and conversions used in the current design.

Table 23. Reaction Conditions and Key Parameters for Lignin BCD

<i>Parameter</i>	<i>Black Liquor</i>
Temperature, °C	120
Pressure, atm	6.32
NaOH loading (minimum required), wt%	5.1% (2%)
Residence time, min	30 min
Total solids ^a , wt %	22.3%
Total solubilization, wt % solids	36%
<i>Deconstruction extents</i>	
Cellulose	48%
Xylan	48%
Arabinan	48%
Lignin	53%

^a Total solids defined as lignin, soluble lignin, cellulose, xylan, arabinan, mannan, galactan, ash, and protein.

Biological funneling occurs through an engineered strain of *P. putida* KT2440, a naturally occurring gram-negative soil bacterium. This strain of *Pseudomonas* is a variant of strains isolated and heavily studied since the 1960s for their novel capability to catabolize aromatics via the β -ketoacid pathway [109-111]. In 2002, the first complete genome was published and expanded the understanding of the aromatic catabolic potential, reigniting interest in its bioremediation applications [112]. Subsequent annotation of the genome pointed to an even more expansive biological toolset including pathways for over 92 compounds (spanning carbon, nitrogen, and phosphorous sources in the natural environment) and physiological mechanisms improving growth under high pH, osmolarity, and the ability to carry strongly oxidative reactions [113]. Work at NREL over the past 4 years focusing on multiple aspects

of the genomic capabilities has led to significant steps forward in the required funneling behavior [114, 115].

In addition to funneling, *P. putida* work at NREL is focused on achieving high selectivity to an adipic acid coproduct. Public literature and patents indicate multiple proposed/known routes to bio-adipic acid from lignin compounds via muconic acid, β -keto adipate, or direct production using an enolase for a final metabolic reduction reaction [116-120]. For this design, aerobic production of muconic acid was selected, which avoids the difficult final reduction reaction, but also has benefits for separations as outlined in further detail below. Specifically, metabolic engineering was used to generate a recombinant strain of KT2440 that prevents lignin catabolic intermediates from entering the central carbon metabolism stopping at cis-cis-muconic acid [121-123]. Additionally, sugar metabolism was modified to divert carbon away from central carbon metabolism and into the upper β -keto adipate pathway, providing a mechanism to valorize multiple substrates to the desired coproduct [121]. Overall, the modeled strain funnels lignin and sugars, as well as long chain acid substrates (e.g., extractives), to muconic acid, with shorter acid species (e.g., acetate) contributing exclusively to growth [124]. The combined effect is to partially decouple growth from production leading to greater overall carbon retention to coproducts than previous attempts. The maximum theoretical metabolic yield of muconic acid as well as product diversion for each substrate were estimated using flux balance analysis on the metabolic reconstruction for the designed strain [125, 126]. The theoretical maximum yield of muconic acid from sugars was estimated as 0.58g/g glucose and 0.59g/g xylose.

As noted in Section 2.1, the “extractives” component in the delivered biomass feedstock represents a significant fraction of the overall biomass, roughly 15 wt%, compared to the lignin fraction at 16 wt%. Although a portion of this component reflects compositional mass balance closures below 100% (representing unknown or unmeasured components), the remainder of the extractives fraction is generally made up of simple components such as sugars, sugar alcohols, and sugar acids, and thus would be readily consumed by *P. putida*. However, given that this can be such a variable component both in the amount and type of extractives present in the delivered biomass feedstock (depending on parameters such as harvest location, time, biomass type, and storage/preprocessing logistics), we did not want to over-credit the TEA by converting all of it to coproduct, nor over-penalize the TEA by ignoring it through the lignin train for it to then add significant COD loading to the wastewater treatment section downstream. Thus, given that whatever level of extractives *do* make it to the facility will be metabolized by *P. putida*, the model treats “extractives” as a long chain acid species, gluconic acid. In the event that extractives could not be utilized at high levels in parallel with solubilized lignin, muconic acid yields would be reduced and residual COD loading to wastewater treatment would be higher (potentially necessitating a move back to including AD in the WWT section as well). In such a case, future plans will investigate other processing alternatives to maintain the \$2.50/GGE MFSP goals including biogas utilization, alternative lignin valorization approaches, and other strategies as outlined at the end of this report in Section 5.4.

The current bioconversion area begins by diluting a subset of the hypertonic BCD solubilized product stream approximately twofold for use in the seed reactors, as well as prefill cycles of production as needed to reduce any osmotic shock experienced by the fermentation organism. Additionally, this attenuates potential toxicity issues with an overly concentrated aromatic stream that are the topic of ongoing research [127]. After this mild conditioning, the feed is cooled to 32°C and a portion of the feed stream is diverted for use in the seed train, where inoculum is grown and concurrently acclimated to the harsher conditions of this fermentation. The seed train uses three stages and begins with a small

0.3 m³ reactor inoculated from the lab, followed by a 1:10 increase to 3 m³. Because an aerobic fermentation enables more rapid growth as well as dense cell cultures compared to an equivalent anaerobic system, a larger 100 m³ third stage with a constant diameter of 2.8 m and a height of 16.8 m or roughly 1/10th the size of the production reactor is used for the final inoculum preparation prior to transferring into the production reactor [128].

Nutrients during the seed reactions include DAP for phosphorus supplementation and host specific nutrients required to properly acclimate the strain to the final feed stream with an assumed cell elemental composition of C₁H_{1.8}O_{0.5}N_{0.2} accounting for the higher intracellular amounts of protein utilized during exponential growth (and associated nitrogen content). The current model assumes only sugars (presumed preferential substrate) are consumed during the seed phases. Table 24 shows the conversions and reactions used in the seed fermentation.

Table 24. Stoichiometry and Conversions Applied for Lignin Bioconversion Seed Train

Reaction	Reactant	% Converted to product
Seed Train:		
Glucose + 0.047 CSL ^a + 0.018 DAP → 6 <i>P. putida</i> _{grow} + 2.4 H ₂ O	Glucose	46%
Glucose + 1.94 O ₂ → 0.74 Muconic + 1.57 CO ₂ + 3.78 H ₂ O	Glucose	54%
Xylose + 0.039 CSL + 0.015 DAP → 5 <i>P. putida</i> _{grow} + 2 H ₂ O	Xylose	46%
Xylose + 1.57 O ₂ → 0.62 Muconic + 1.26 CO ₂ + 3.13 H ₂ O	Xylose	54%
Arabinose + 0.039 CSL + 0.015 DAP → 5 <i>P. putida</i> _{grow} + 2 H ₂ O	Arabinose	46%
Arabinose + 1.57 O ₂ → 0.62 Muconic + 1.26 CO ₂ + 3.13 H ₂ O	Arabinose	54%

^a CSL and DAP are both nitrogen sources required for growth. The stoichiometry shown above is only used to balance the compositions assumed for cell mass.

Building on extensive studies and experience with aerobic fermentation reactor modeling developed during prior work and bench-scale runs supporting aerobic lipid production (detailed previously in section A500), the remaining feed is sent to supply large production reaction bubble columns shown in Figure 14.

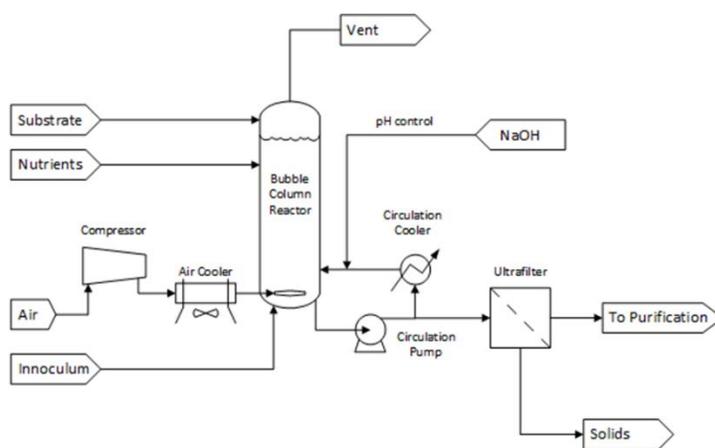


Figure 14. Aerobic bubble column bioreactor setup

A pressurized air stream is sent to a sparger at the base of the column. As the gas travels upwards bubble expansion and hydrodynamics promote mixing and mass transfer throughout the two-phase system. Compared to stirred tank reactors that use motor speed to achieve sufficient mixing and control the sparge rate to achieve sufficient gas transfer, bubble columns only provide a single control, the gas sparge rate, to achieve both mixing and mass transfer. Despite this drawback in flexibility, at larger volumes bubble columns provide more cost-efficient oxygen delivery as well as reduced shear on the organism due to absence of mechanical components [13]. Additionally, the simpler mechanical design aids in aseptic operation. To date, the TEA models assume standard bubble column designs outfitted with air sparge rings at the bottom of the columns; however, more advanced designs may be possible to aid in improving oxygen mass transfer at lower aeration rates (such as advanced baffle designs, microfine bubble sparging, air input port placement, etc.), which may be considered in the future. Recent NREL work has begun to investigate such implications across different design configurations through computational fluid dynamics (CFD) modeling, which may be leveraged in the future to further optimize aerobic bubble column design.

To meet the higher heat demands associated with aerobic fermentation, each column is outfitted with a pump-around cooling loop running through a chilled-water heat exchanger. Previous design reports indicated the importance and outlined in greater detail the traditional equations used to estimate mass transfer in stirred tank reactors. In the current model, a correlation relating the superficial velocity, temperature, and viscosity of the fluid to the overall mass transfer coefficient in a bubble column is used in combination with Henry's law and the oxygen partial pressure of the gas at the top and bottom of the bubble column to explicitly determine the OTR [129]. The necessary amount of pressurized air delivered to the system is then determined such that the OTR is equivalent to the OUR, assuming all oxygen delivered to the liquid phase is available to the organism without transport limitations. Equation 1 shows the correlation and oxygen transport rate equations used in the model [129]:

$$\begin{aligned}
 k_L a &= 0.32 (u_s)^{0.7} (\mu_{eff})^{-0.84} \times 1.025^{(T-20)} \\
 \text{OUR} = \text{OTR} &= k_L a (C^* - C_L)_{\text{MEAN}}
 \end{aligned}
 \tag{1}$$

Nutrients supplied during the seed reactions include DAP for phosphorus supplementation and ammonia to provide sufficient nitrogen to the strain. The production reaction occurs over a longer period (not exclusively focused on growth and acclimation) and the cell is expected to enter a stationary phase. To account for the slower specific growth rate and lower nitrogen demand accompanying stationary phase the cell elemental composition is assumed to be $C_1H_{1.85}O_{0.828}N_{0.058}$ during the production reaction. The net metabolic stoichiometry and conversion of the muconic acid fermentation is a combination of theoretical maximum metabolic yields and maintenance/respiration reactions dependent on the specific substrate consumed. While it is likely regulatory effects will initially cause a substrate diauxic preference, where one carbon source may be consumed prior to others, it is assumed the target strain will be sufficiently engineered to co-consume 98% of the carbon sources over the course of a fill/draw cycle and avoid large carbon losses to the exiting broth. For the production reaction, Table 25 lists the biological reactions and conversion to product for the carbon sources in the feed stream.

Table 25. Stoichiometry and Key Conversions for Bioconversion of Lignin and Residuals

Reaction	Reactant	% Diverted to product
Production Reactor:		
Glucose + 1.18 O ₂ + 0.28 NH ₃ → 4.8 <i>P. putida</i> + 1.2 CO ₂ + 1.98 H ₂ O	Glucose	46%
Glucose + 1.94 O ₂ → 0.74 Muconic + 1.57 CO ₂ + 3.78 H ₂ O	Glucose	54%
Xylose + 0.98 O ₂ + 0.23 NH ₃ → 4 <i>P. putida</i> + 1 CO ₂ + 1.64 H ₂ O	Xylose	46%
Xylose + 1.57 O ₂ → 0.62 Muconic + 1.26 CO ₂ + 3.13 H ₂ O	Xylose	54%
Arabinose + 0.98 O ₂ + 0.23 NH ₃ → 4 <i>P. putida</i> + 1 CO ₂ + 1.64 H ₂ O	Arabinose	46%
Arabinose + 1.57 O ₂ → 0.62 Muconic + 1.26 CO ₂ + 3.13 H ₂ O	Arabinose	54%
Sucrose + 2.35 O ₂ + 0.56 NH ₃ → 9.6 <i>P. putida</i> + 2.4 CO ₂ + 2.96 H ₂ O	Sucrose	46%
Sucrose + 3.8731 O ₂ → 1.48 Muconic + 3.13 CO ₂ + 6.57 H ₂ O	Sucrose	54%
Acetate + .39 O ₂ + 0.093 NH ₃ → 1.6 <i>P. putida</i> + 0.4 CO ₂ + 0.66 H ₂ O	Acetate	100%
Extractives + 0.68 O ₂ + 0.28 NH ₃ → 4.8 <i>P. putida</i> + 1.2 CO ₂ + 1.98 H ₂ O	Extractives ^{a,b}	46%
Extractives + 1.44 O ₂ → 0.74 Muconic + 1.57 CO ₂ + 3.78 H ₂ O	Extractives ^{a,b}	54%
Lignin + 3 O ₂ → 1 Muconic + 2 CO ₂ + 1 H ₂ O	Lignin monomer	100%

^aExtractives are assumed to be gluconic acid, which metabolically behaves similarly to glucose as a C₆ carbon substrate.

^bOn a mass basis biomass yield from extractives = 0.314 g/g extractive, muconic yield = 0.289 g/g extractive

The fermentation is run in a fed batch mode, with an assumed average working volume of 70%. Broadly, the reactor is prefilled with diluted feed to ~50%, then the inoculum is transferred to the reactor. The reactor is then filled adjusting the rate of the concentrated feed to maintain a low but nonlimiting amount of carbon, which also improves the volume use over the course of the fermentation. When the maximum working volume of the column is reached, a portion of the broth is drawn, then fed batch operation proceeds. This cycle repeats for the duration of the fermentation, then the full volume of the reactor is drained.

The fermentation is controlled at a constant temperature of 32°C and operates at a mild positive pressure of 1.34 atm, which assists in maintaining the axenic process. The current process assumes 1,000 m³ reactors with a length-to-diameter ratio of 6 translating to a diameter of 6 m and height of 35.8 m. Overall, to completely convert the feed stream requires 17 bubble columns that are fed by 3 separate seed trains. Because the muconic acid product is an acid, it is necessary to consider the impact of pH during the fermentation. While evidence exists of *P. putida* tolerance in the basic environments more commonly found in soil environments (particularly if acclimated over a longer time), the inverse—tolerance to acidic conditions—is less well documented. To address this gap, the current design implements pH control to neutralize the acid produced during the fermentation (as needed in excess of the caustic in solution) administered in the pump-around loop after cooling the broth. The overall fermentation is targeted to occur at a net productivity of 1 g muconic acid/L/hr across all consumed substrates. The current model predicts net (i.e., including drawn volume/broth) cell titers at the end of the fermentation of 38 g/L, and muconic acid titers of 68.5 g/L. Table 26 lists the major reactor specifications for the seed and production system.

Table 26. Key Operating/Design Parameters for Lignin Seed and Production Bioreactors

<i>Parameter</i>	<i>Value</i>
Seed train	
Temperature, °C	32
Pressure, atm	1.34
Stage 1 volume	0.3 m ³ (80 gallon)
Stage 2 volume	3 m ³ (800 gallon)
Stage 3 volume	100 m ³
Diameter	2.8 m
Height	16.8 m
Number of seed trains	3
Production reactor	
Temperature, °C	32
Pressure, atm	1.34
Volume	1,000 m ³
Diameter	6 m
Height	35.8 m
Net fermentation productivity, g/L/hr	1
Net cell titer, g/L	38
Net muconic acid titer, g/L	68.5

After the fermentation, the collected broth is sent through an ultrafilter to remove debris and cell mass. The remaining solids are sent to wastewater treatment and eventually burned in the high-solids boiler. The recovered liquid is carbon filtered to remove coloring compounds then proceeds to the muconic acid recovery system. The muconic acid is acidified and recovered via low temperature crystallization in the acid form [122]. Existing and predicted solubility curves for muconic acid and adipic acid shown in Figure 15 illustrate the strong temperature dependency of solubility for the fully protonated species [130, 131]. At temperatures above the freezing point of water, fully protonated muconic acid (and adipic) will crystallize forming a high purity solid phase that can be easily removed via centrifugation from the residual liquid broth. However, compared to adipic acid, the muconic acid is on the order of ~10 times less soluble at equivalent temperatures and crystallizes to near completion with minimal loss increasing carbon efficiency.

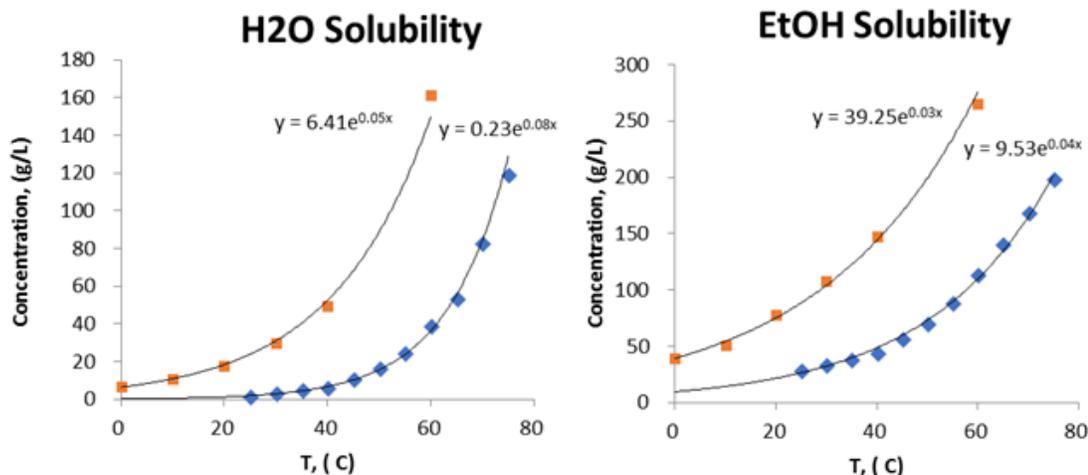


Figure 15. Predicted solubility curves for muconic and adipic acid

The current design assumes reacidification using sulfuric acid to drop the pH to 2, where the muconic acid is in the protonated form. Rigorous pH calculations were performed at the predicted crystallization feed conditions and muconic acid pKa to understand the significance of pH variations, and it was determined that a pH of 2 should sufficiently ensure greater than 98% of the dissolved muconic acid will be in the protonated form. Because the second pKa of muconic acid is not well measured or reported, it was estimated using the second pKa of adipic acid ratioed by quotient of the first pKas. While this is not an accurate approach, at the low pH in the current design errors of $\pm 20\%$ have minimal effect on the overall recovery. Figure 16 shows the species equilibrium as a function of pH.

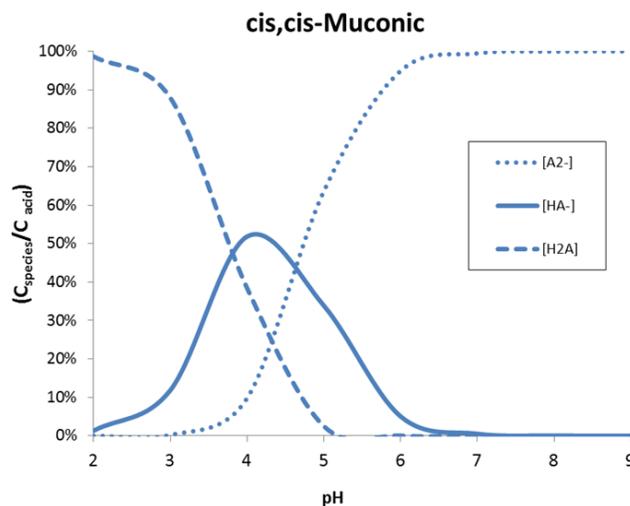


Figure 16. Acid-base equilibrium species at a given pH

The crystallization occurs at a temperature of 15°C , and a pH of 2, recovering 98.8% of the product. The recovered crystal contains minor amounts of salt and water entrained in the crystal. The crystallizer mother liquid/broth is re-neutralized then sent to wastewater treatment where the salt is eventually separated and disposed of. The entrained liquid in the crystal is removed via a fluidized-bed

drier, and then re-dissolved into an ethanol solvent. The ethanol:muconic acid ratio is set at 4 constrained to remain above the solubility limit of muconic acid in ethanol (Figure 14) at the mixing vessel temperature. Upon dissolution, the entrained salt ions precipitate out of the ethanol and are filtered prior to muconic acid upgrading. Table 27 lists the key crystallizer metrics.

Table 27. Muconic Acid Crystallizer Metrics

<i>Parameter</i>	<i>Value</i>
Acid-base chemistry	
pKa ₁ muconic acid	3.87
pKa ₂ muconic acid (estimated)	4.726 (~3.87/4.43*5.41)
pKa ₁ adipic acid	4.43
pKa ₂ adipic acid	5.41
pKa ₁ H ₂ SO ₄	-3
pKa ₂ H ₂ SO ₄	1.99
Muconic acid crystallizer operation	
Target pH	2
Temperature, °C	15
Pressure, atm	1
Percent recovery	98.8%
ppm salt contamination	13,400
Configuration	Oslo continuous crystallizer

Adipic acid upgrading occurs in the liquid phase in a three-stage packed bed reactor operating at 40 atm. Hydrogen is fed in excess at a molar ratio of 2.6 mols H₂:mol muconic acid to ensure complete hydrogenation. The reactor is operated at a mild temperature of 78°C to avoid cracking of the facile double bond backbone, as well as over hydrogenation of the acid end groups critical to the final polymer properties. Inter-stage cooling is used to minimize temperature rise across each bed associated with the exothermic hydrogenation reactions. Complete hydrogenation is modeled based on experimental results over a 2% ruthenium on carbon catalyst [122, 123]. After hydrogenation, the vapors are flashed and sent to the combustor, with the liquid proceeding to a flash evaporator which concentrates the adipic acid to a ratio of 2.5 ethanol:adipic by mass at elevated temperatures. The concentrated adipic acid product stream is crystallized by lowering the temperature to 15°C [132, 133]. 73.4% of the adipic acid is removed per pass as crystals via centrifugation, and the mother liquor with the remaining uncrystallized adipic acid and ethanol is recycled back to the evaporation cycle until extinction. The recovered crystal product is sent to a drier to remove entrained ethanol, then stored on-site. Table 28 lists the key design parameters for the hydrogenation reactor and adipic acid crystallizer.

Table 28. Muconic Acid Upgrading to Adipic Acid and Adipic Acid Recovery

<i>Parameter</i>	<i>Value</i>
Hydrogenation reaction	
Ethanol:Muconic acid mass ratio	4
Temperature, °C	78
Pressure, atm	40
H ₂ :Muconic molar ratio	2.6
Muconic acid conversion	100%
Catalyst	2% Rh/C
WHSV (feed mass flow/catalyst mass)	5 hr ⁻¹
Adipic acid crystallizer operation	
Configuration	Oslo continuous crystallizer
Ethanol:Adipic ratio feed	5.3
Ethanol:Adipic ratio concentrated	2.5
Crystallization temperature, °C	15
Pressure, atm	1
Single-pass adipic acid recovery	73.40%

3.7.3 Cost Estimation

The BCD process occurs in a 127 m³ pulping reactor vertical pressure vessel with a design similar to the pre-steaming section of the dilute acid pretreatment reactor [10]. The vessel metallurgy was designed using 316 stainless steel as the material of construction with the appropriate vessel wall thickness for the elevated pressure.

All fermentation units are constructed of 304 or 316 stainless steel. Stainless steel is necessary to achieve the corrosion resistance to caustic solutions, as well as axenic fermentations where cleaning, contamination, and improved weldability are important considerations. The initial two seed fermentors maintained the same cost basis as the 2011 design report, quoted by A&B Process Systems Corp. as skidded units with cooling jackets and agitators included. The third seed unit and production unit are bubble column reactor units with a length-to-diameter ratio of 6 (100 m³ unit: 35.8 m height, 6m diameter) estimated through a combination of industry quotations and ACCE cost modeling. The bubble column reactors are sized to include a headspace allowance for expansion and vapor disengagement and use a pump-around loop to maintain the proper fermentation conditions. Fermentation compressors were sized based on the required air flow rate for meeting the OUR demands, with a pressure increase determined by the reactor dimensions and hydraulic pressure at the bottom of the broth (~45 psig). Air compressors were constructed of carbon steel owing to the lack of corrosive chemical components.

Ultrafiltration and carbon filtration units were estimated based on guidance from an engineering consultancy with Nexant and designed as a counter current diafiltration package unit including feed pumps and controls. The unit is sized for a base membrane area of 53,820 ft² and includes an operating cost for membrane replacement. The carbon filtration unit has two beds and is constructed of carbon steel with stainless steel cladding to resist the corrosive acidic solution. The process stream flows through the first, while the second is regenerated using high pressure steam. The cycle time for each bed is assumed to be 1 hour. Granular active carbon was costed separately and replaced assuming a 3-year lifetime.

The crystallizer, centrifuge, and crystal drier unit capital costs were scaled from estimates provided by Nexant. The muconic acid crystallizer is designed as a continuous two-stage process occurring in Oslo type units that implement circulation cooling loops to maintain the constant temperature control required for the process. To recover high amounts of muconic acid a chilled-water heat exchanger was used, and the heat of reaction due to pH adjustment is accounted for. The muconic crystal recovery centrifuge operates continuously with a wash. Crystal dryers are designed as fluidized-bed units that circulate filtered hot air over the crystals (based on the information provided by Nexant). The design includes two parallel units sharing a single hot air unit.

The adipic acid hydrogenation reactor was quoted as a low-pressure fixed bed hydrodeoxygenation unit. The base reactor price quote was estimated through a separate NREL study of existing hydrotreater facility capital costs and correlations to liquid feed volume flow [134-142]. The base conditions for the hydrotreater estimate, pressures >1,000 psig and temperatures >370°C, were de-escalated using the Guthrie pressure factor approach and the reactor size was scaled according to the total liquid volume (ethanol and muconic acid) entering the reactor[139]. Inter stage coolers, economizer heat exchangers, combined heat and power (CHP) systems, flash separators, and pumps were costed using ACCE[103]. In addition, the five-stage reciprocating makeup hydrogen compressor with a backup spare unit was costed using ACCE.

The adipic acid concentrator was designed as an initial mixing/feed tank, followed by a heat exchanger and flash evaporation tank constructed of SS316 for additional corrosion resistance. Adipic acid crystallizers, centrifuges, and dryers assumed similar designs as the muconic acid unit but scaled to the proper product stream.

3.7.4 Achieving the Design Case

Lignin conversion to value-added chemicals and materials has substantial promise to improve the overall economics of a lignocellulosic biorefinery, beyond its value as a boiler fuel. Moreover, the valorization of lignin is a critical need for ultimately enabling the lignocellulosic bioeconomy given that it can comprise up to a third of the carbon in plant biomass. This problem is incredibly challenging and has been actively researched for at least a century, with only a few options to date being economically viable, primarily including vanillin and lignosulfonates.

The approach described here, namely the use of a lignin depolymerization technology—a microbe to funnel a heterogeneous mixture of lignin-derived compounds to a single intermediate—and catalytic upgrading to a final product is a relatively new and potentially promising approach to valorize lignin [107, 114, 143], but multiple technical challenges remain. The process modeled here uses BCD as a baseline approach for lignin depolymerization; this method has long been studied, but at low severity the monomer yields remain too low and at high severity the stream becomes quite toxic for microbial conversion. Broadly, one of the key limitations to date with a general approach of an intermediate biological step is the lack of robust catalytic technologies to depolymerize multiple bond types in lignin and provide sufficient bioavailable lignin-derived monomers. Specifically, aryl-ether bond cleavage is relatively well-known chemistry—for example, via reductive or oxidative routes [106, 144]—but lignin from most bioenergy feedstocks also exhibits a high fraction of C-C bonds. Developing robust catalytic technologies to cleave both C-O and C-C bonds in lignin will be critical to ensuring a high yield of bioavailable compounds, one of the key limitations in reaching high yields of final products.

In terms of the metabolic engineering aspects, substantial work remains in the development of robust microbes that are tailored to the lignin stream of interest for valorization. Significant efforts are now going into this problem worldwide, primarily via the use of non-model strains that harbor native aromatic catabolic capacity, such as *P. putida*, *Rhodococci*, and others. The process-relevant parameters of titer, rate, yield, and product recovery are of course key cost drivers. Similar to sugar conversion using pretreated hydrolysates, but likely more acute, aromatic compounds are typically quite toxic to microbes, and thus another important research area in this vein is in improving robustness of the chassis of choice for biological funneling. Beyond this, these types of streams may contain not only lignin, but also high content of extractives, sugar degradation products, or even sugars. Expanding the capacity of a microbe to truly convert all of these products into a single intermediate in an atom-efficient way remains a considerable challenge. While the current design implements a monoculture, the opportunities here for co-cultures or mixed cultures are considerable as well. Additionally, in the presence of solubilized lignin oligomers, some aromatic-catabolic bacteria have been shown to be able to depolymerize oligomers [143], but the mechanisms for this also remain unknown. The interface between the upstream catalysis and the microbial conversion step, overall, remain an area of active and intense investigation and likely will be the critical driver for the long-term viability, or lack thereof, of a biological lignin valorization approach.

Beyond the use of a microbial conversion step, the concept of a “lignin-first” biorefinery has emerged in the last decade [106, 144]. One variation of this approach pursued at NREL, dubbed “reductive catalytic fractionation,” or RCF, uses a polar protic solvent, such as methanol, at high temperatures to selectively solubilize lignin from whole biomass and passes it over a reducing catalyst in the presence of hydrogen or a hydrogen donor (such as a secondary alcohol or hemicellulose-derived sugars). RCF has created excitement in the lignin valorization community because it is an active stabilization method that can be tuned to yield complete aryl-ether bond cleavage and a narrow slate of aromatic monomers and easily digestible, delignified polysaccharides. RCF chemistry also holds promise for non-thermochemically pretreated biomass in which the polysaccharides have been removed, but where aryl-ether linkages are still intact. Multiple challenges remain for this approach to become viable and TEA will be critical to determine the primary cost drivers for these and any alternative approaches for lignin valorization.

Finally, the last decade has seen considerable improvements in the genetic engineering of bioenergy crops [144, 145]. The overall outcome of these studies has been to demonstrate that lignin chemistry *in planta* is plastic and can be tuned in a way that maintains the efficacy of the overall plant. Even though ideally lignin valorization solutions will be developed that are feedstock agnostic, the variation in lignin chemistry between softwoods, hardwoods, and grasses is considerable, and even lignin chemistry variation within undomesticated species can be quite broad. Ideally, and in the long term, dedicated bioenergy crops will be selected and grown that not only maximize biomass and sugar yields, but also that have ideal lignin for valorization purposes while still achieving net improvements in sustainability.

3.8 Area 800: Combustor, Boiler, and Turbogenerator

3.8.1 Overview

The purpose of the combined heat and power (CHP) subsystem is to burn various organic byproduct streams to produce steam and electricity. Combustible byproducts include unconverted lignin and carbohydrates from the feedstock, cell mass from fermentation and WWT, and off-gas streams from catalytic upgrading operations. Combustion of these byproduct streams generates steam to drive the upgrading and separation operations, and partially offsets the plant's electric power demand. It also reduces solid waste disposal costs and satisfies any regulatory issues with the handling of genetically engineered organisms.

Compared to previous biochemical design reports, the case for an integrated CHP system in the present design is less strong. In earlier designs, combustion of the unconverted lignin and extractives fractions provided (in many cases) sufficient heat and power to drive the entire process, with some excess power that could be exported as a coproduct. With the inclusion of lignin fermentation and upgrading technology in the present design, combined with the associated loss of extractives in the lignin fermentation process, the amount of residual solid fuel left for combustion is significantly reduced, and anaerobic digestion biogas is eliminated (because the anaerobic digestion unit is removed). Still, because there are residual waste solids still remaining after the lignin upgrading process as well as wastewater sludge (which would create a disposal problem if they could not be combusted on-site, including the use of engineered organisms), and because of the continued need for utility steam heating, the CHP area was retained in the present design and includes the same unit operations as before. Moreover, there is considerably higher use of sodium throughout the facility (i.e. DMR pretreatment, BCD lignin deconstruction, muconic acid fermentation, and ion exchange regeneration), the majority of which goes to WWT as soluble salts, but it is likely that sodium levels reaching the boiler with cake solids will also be higher than prior designs, increasing the risk for boiler slugging. Thus, if the solids boiler continues to be maintained in future designs, these issues must be further investigated with inputs from engineering subcontractors or boiler vendors. Accordingly, Area 800 remains an area for future optimization and cost reduction.

The fuel streams are fed to a combustor capable of handling the wet solids. A fan moves air into the combustion chamber. Treated water enters the heat exchanger circuit in the combustor and is boiled and superheated to high-pressure steam. A multistage turbine and generator are used to generate electricity. Steam is extracted from the turbine at two different conditions for use in the process. In the final stage of the turbine, the remaining steam is taken down to a vacuum and condensed with cooling water for maximum energy conversion. The condensate is returned to the boiler feed water system along with condensate from the various process heat exchangers. The steam turbine turns a generator that produces AC electricity for all users in the plant. NO_x emissions are mitigated with ammonia injection in a selective non-catalytic reduction (SNCR) system, and SO_x emissions are mitigated with flue-gas desulfurization.

3.8.2 Design Basis

The 2011 design report presented a CHP system comprising a high-solids, bubbling fluidized-bed boiler raising high-pressure (HP) steam at 900 psig, and a condensing steam turbine with two steam extractions at 175 psig and 125 psig. The boiler was based on the Babcock & Wilcox Towerpak product, which is only able to raise steam at a single pressure. In both the acids and the BDO cases, the upgrading and distillation operations after fermentation required significantly higher temperatures than

were specified in the previous design reports. In the acids case, some of the process temperatures were impossible to reach with steam at any pressure, so fired heaters were specified, with HP steam preheat and trim. In the BDO case, however, the oligomerization reactor requires a significant amount of heat at 250°C. This is well served by 900 psig steam and consumes about 40% of the total steam thus produced. At this pressure, piping becomes more expensive and it is optimal to locate the process nearby the boiler to minimize piping runs; this is a consideration beyond the engineering feasibility level of analysis in the present design, but is worth noting for future work. An alternative could be a similar hot oil system or natural gas-fired heaters, which may be a more practical solution but would require consideration of LCA tradeoffs given high heat demands required for these heaters.

Apart from the limited number of HP steam users, the next level of steam required in either process is 175 psig, which is used for heating biomass feed to pretreatment temperatures by direct injection. Because the boiler is limited to a single steam pressure, and because both cases require some 900 psig steam, the steam turbine and electrical generator from earlier designs were retained to capture some energy from this pressure reduction. In future designs of the acid case, the relatively small trim duties could be absorbed in the specified fired heaters and the production of HP steam could be eliminated, reducing the boiler and feed water treatment capital costs, with the tradeoff of slightly higher natural gas costs. The BDO case is not so straightforward, given the high HP steam duty requirement of the oligomerization reactor. A fired heater or secondary HP boiler operating on natural gas could be used here as well, but the capital and operating cost tradeoffs are more difficult to determine, given the efficiencies of each. Ultimately, this is a minor sensitivity compared to other uncertainties in either process so, for simplicity and comparison, the CHP system was left the same as in previous design reports.

The details of the CHP system design can be found in the 2011 report. To briefly summarize, the design uses a bubbling fluidized-bed combustor capable of complete combustion of the wet solid fuel and gas streams, along with any supplemental natural gas. Flue gas from the combustor preheats the entering combustion air then enters a spray dryer for flue gas desulfurization (FGD). Ash is removed in a baghouse and disposed to a landfill. Finally, the boiler raises steam at 900 psig, which is superheated and then sent through a multistage steam turbine with two extraction ports and a final condenser. The steam turbine turns an electric generator to offset some of the power demand in the process. The balance of electric power is assumed to be purchased from the grid (see Area 900).

3.8.3 Cost Estimation

For the 2011 design report, Harris Group worked with Babcock & Wilcox and Siemens to provide capital cost quotes for the biomass boiler and condensing extraction turbine and generator. The cost basis for the A800 equipment remains the same as described in the 2011 ethanol report. The boiler capital cost includes the boiler feed water preheater, FGD spray dryer, and baghouse. For the baghouse, bag replacement appears as a periodic charge in the cash flow worksheet. Harris Group also obtained quotes from a third vendor for support equipment including the deaerator, chemical injection system, tanks, and pumps.

3.9 Area 900: Utilities

3.9.1 Overview

Area 900 tracks all plant utilities except steam, which is provided by Area 800, including electric power, cooling water, chilled water, plant and instrument air, process water, and the CIP system. The process water manifold in Area 900 mixes fresh water with treated wastewater and condensate from the sugar evaporation system (assumed suitable for all plant users) and provides this water at a constant pressure to the facility. Water is provided to the cellulase production unit, boiler and cooling tower makeup, the CIP system, and the wash for the lignin filter press. Fresh water is also mixed with some internally recycled water for dilution before pretreatment and enzymatic hydrolysis. The plant and instrument air systems provide compressed air for general use (pneumatic tools and clean-up) and instrument operation. Larger users of compressed air, namely the cellulase system and aerobic bioreactors, have their own compressors specified. The CIP system provides hot cleaning and sterilization chemicals to hydrolysis, bioconversion, and the enzyme production section.

3.9.2 Design Basis

The cooling water system is designed for a 28°C supply temperature with a 9°C temperature rise in coolers throughout the facility. This is an assumed average rise; the actual cooling water rises across each exchanger are not explicitly modeled in Aspen. The primary cooling water users option are described in Table 29, and their contributions are compared in Figure 17.

Table 29. Major Cooling Water Users

Evaporator condensate cooler	Provides cooling of the sugar evaporator condensate (acids case only).
Lignin upgrading coolers	Trim cooling duty used in the lignin conversion/upgrading area.
Turbine condenser	Condenses the steam turbine exhaust at a vacuum.
Chiller condenser	The chilled-water loop requires cooling water to condense the refrigerant. The cooling water duty to M-908 is set equal to the total load on the chilled-water loop. In Figure 17, the chiller contributions are divided by area.

As noted in Section 3.8, the heat and power balance has changed significantly since the 2013 design report, so the condensing turbine is no longer the largest user of cooling water. In fact, the steam system becomes heat limited for the more heat-intensive BDO pathway (associated with energy demands around aqueous BDO upgrading) and must import natural gas to satisfy facility heat requirements, leaving minimal steam routed through the final condensing turbine stage. The single largest user is the chiller condenser, which services the chilled-water loop used in Areas 300, 400, and 700, driven primarily by Area 700 cooling demands; at the cooling temperatures dictated in Area 700, it would be difficult to avoid chilled water utilities for this section. The compressor electricity demand for the chiller was estimated at 0.56 kW/ton of refrigeration and the cooling water demand for the chiller system was assumed to be equal to the heat removed in the chilled-water loop.

The cooling tower evaporation rate is based on a temperature drop from 37°C to 28°C. Windage was taken to be 0.005% of the total flow to the tower and cooling tower blowdown was assumed to be 0.15% of the flow leaving the tower basin.

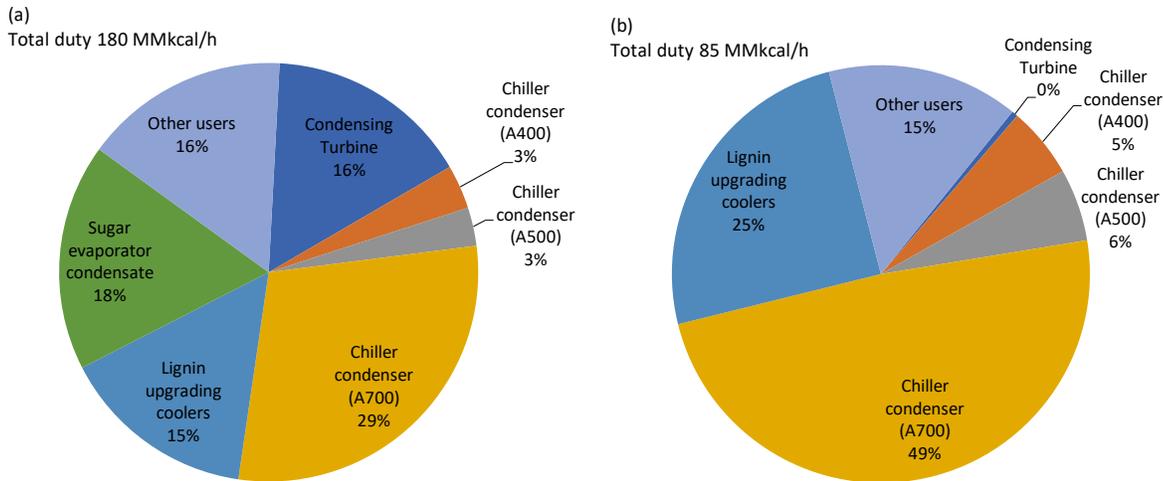


Figure 17. Cooling water heat duty distribution between major users; (a) acids case, (b) BDO case

Fresh water is assumed to enter the facility at 13°C and provides supplemental cooling to the plant before entering the process water tank. The fresh water is mixed with the treated wastewater effluent and the evaporation condensate in the process water tank (T-914) and then split several ways. Clean water must be provided to biomass dilution in the front end, to the cellulase production unit, to the washing filters, and to the boiler and cooling tower water makeup. The process water tank is designed for an 8-hour residence time. The process water pump (P-914) pumps water from the tank into the facility and is designed to handle 1.5 times the process water flow requirement.

The plant and instrument air systems provide compressed air for pneumatic tools and clean-up and instrument operation (not including major air demands such as enzyme and product bioreactors). The plant air compressor is sized for 400 SCFM at 125 psig. An instrument air dryer and surge tank were designed to provide clean dry air at a consistent pressure to the instrument air system. The surge tank was sized at 3,800 gallons.

The electricity generated in Area 800 is used to partially offset the plant power demand throughout the facility to power pumps, agitators, compressors, etc. (65.2 MW total power required for the acids case and 54.2 MW for the BDO case), but there is still a considerable power deficit on the order of roughly 42–44 MW that must be imported from the grid after considering the power generated on-site. The distribution of total plant power utilization among all areas is shown in Figure 18. Note that the cost of the power required by Area 100 is already assumed to be included in the feedstock cost and is subtracted from the plant's net electricity import. This is reflected in the economics by an operating cost credit equal to this amount of electricity.

In both pathways, Area 200 constitutes a sizeable power demand, primarily due to the switch to DMR pretreatment in this design, which trades heat demands that were required more substantially for DDA pretreatment with power demands to drive the mechanical refining equipment. Additionally, Area 300 constitutes a large power consumer for the acids pathway, primarily due to the addition of continuous enzymatic hydrolysis and subsequent MVR evaporation units (dictated most strongly by the latter,

with MVR evaporators driven by power rather than heat). In the future, steam rather than MVR evaporators may be further considered for cost versus energy usage tradeoffs.

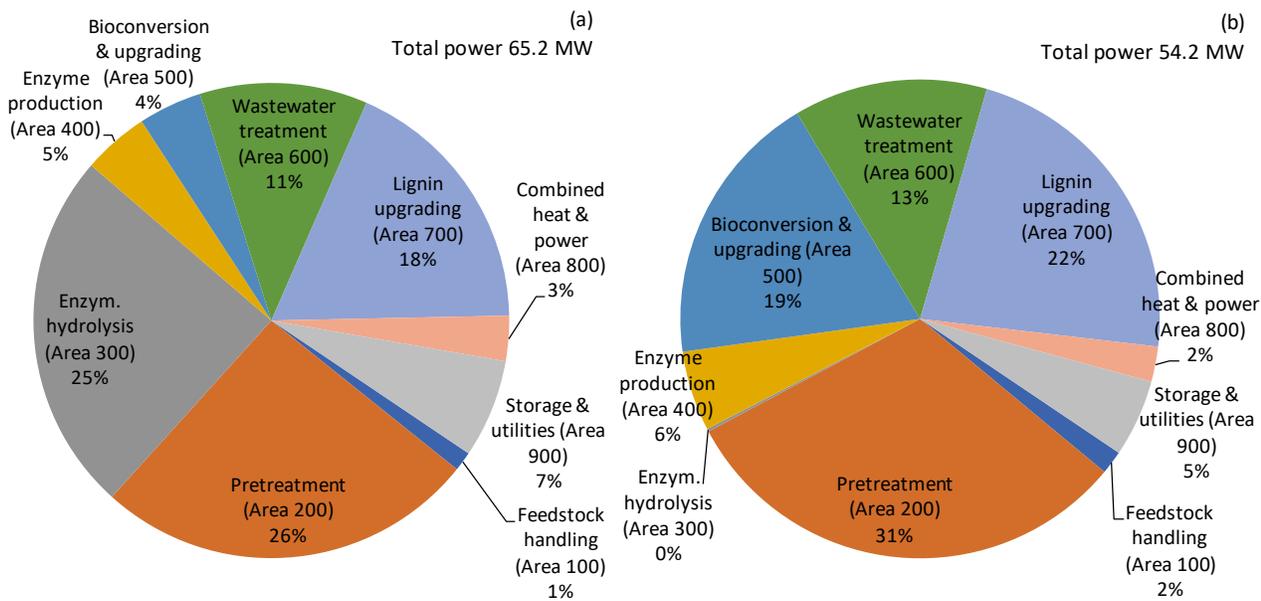


Figure 18. Distribution of plant electricity utilization by process area; (a) acids case, (b) BDO case

3.9.3 Cost Estimation

All cost estimates for the utility equipment in A900 were maintained consistent with the basis values used in the 2011 report. To summarize, the cooling tower was based on a cost estimate from a vendor for a fiberglass cooling tower capable of handling 44,000 gal/min; this cost is scaled to the respective cooling water throughputs estimated here. Harris Group had estimated costs for the cooling water circulation and makeup pumps using their internal database. The material of construction for the cooling water loop is carbon steel. The cost for the chiller came from a recent quote for a similarly sized system. Harris Group had also used their internal database to estimate costs for the remaining equipment: the process water tank and pump; the plant/instrument air compressor, dryer, and surge tank; and the CIP system.

4 Process Economics

The ultimate purpose for developing such a detailed process design, simulation model, and cost estimate is to determine the economics of biofuel production in an integrated biorefinery. This information is used either as an absolute cost to assess the product's potential in the marketplace or as a relative cost that can be used to guide research by examining the change in production cost associated with a process modification or other core research activity.

The total capital investment (TCI) is first computed from the total equipment cost (estimated per above based on process flows which allow for designing/sizing all equipment and associated capital costs). Next, variable and fixed operating costs are determined. With these costs, we use a discounted cash flow analysis to determine the minimum fuel selling price required to obtain a zero net present value (NPV) with a fixed internal rate of return (IRR). This section summarizes the assumptions made in completing the discounted cash flow analysis, with more details and supporting description available in the 2011 ethanol design report [2] and 2013 biological hydrocarbon design report [10] for assumptions that are unchanged. Our analysis does not take into account any policy factors such as subsidies, mandates, or carbon credits, because these would be speculative. The purpose of this analysis is to demonstrate the process requirements needed to achieve specific DOE cost targets which are set from the top down, and to demonstrate how the technology pathway described here is able to achieve such targets on its own merits (through bottom-up TEA modeling) and, if it cannot, to give stakeholders a sense of the magnitude of incentive required to make it so.

4.1 About Cost-Year Indices

The cost-year of 2016 was chosen for this analysis to provide more updated and relevant cost output information relative to prior efforts in 2011\$ and 2014\$ [10, 146]. This new basis is being applied consistently across all DOE-BETO platforms for which similar design case target projections are being established to support upcoming Multi-Year Program Plan (MYPP) efforts, to permit comparison of future feedstocks, conversion technologies, and other alternative scenarios. However, equipment and material costs are largely based on information obtained in previous years, which must then be indexed to 2016. As presented in prior design cases and MYPP reports [2, 146], capital costs were adjusted using the Plant Cost Index from *Chemical Engineering Magazine* [147] to a common basis year of 2016. Similarly, for chemical/material costs we used the Producer Price Index (PPI) for chemical manufacturing published by the U.S. Bureau of Labor Statistics [148]. Employee salaries were maintained from prior basis values and were scaled to 2016 using the labor indices provided by the U.S. Bureau of Labor Statistics [148]. The general formula for cost-year dollar back-casting is:

$$2016 \text{ Cost} = (\text{Base Cost}) \left(\frac{2016 \text{ Cost Index}}{\text{Base Year Index}} \right)$$

4.2 Total Capital Investment

Section 3 of this report describes the details of the conceptual process designs and how the purchased cost of the equipment was determined. The next step is to determine the installed cost of that equipment. The installation cost can be determined by performing a detailed study of everything required to install the necessary equipment and make it operational (e.g., foundation, piping, and wiring). This type of detail is not warranted at this level of process development, and a factored approach in which multipliers are applied to the purchased equipment cost is considered satisfactory.

The methodology and rationale for applying unit-level installation costs remain the same as described in the 2011 and 2013 reports, and again, further detail can be found there that will not be repeated here.

In summary, each type of equipment utilizes a different installation factor to scale the given direct equipment purchased cost to a final installed cost. A complete list of the equipment is provided in Appendix A, along with equipment purchased and installed costs. The purchased cost for a given component reflects a baseline equipment size. As changes are made to the process, the equipment size required may be different than what was originally designed and costed. Instead of re-costing in detail, an exponential scaling expression was used:

$$\text{New Cost} = (\text{Base Cost}) \left(\frac{\text{New Size}}{\text{Base Size}} \right)^n$$

In this equation, the scaling exponent n varies depending on the type of equipment to reflect economy-of-scale dependencies (more detail on reasonable scaling values for different types of equipment is provided in the 2011 ethanol report [2]). The basis for scaling is typically some characteristic of the equipment related to production capacity, such as flow or heat duty. Some equipment does not follow, such a scaling-factor approach, namely when the capacity for a given operation is exceeded and requires multiple units in parallel, thus losing economy-of-scale benefits that are captured in the exponential expression above.

Once the total equipment cost has been determined in the year of interest, several other direct and indirect costs were added to determine the TCI. Site development and warehouse costs, along with additional piping, are based on the inside-battery-limits (ISBL) equipment costs (Areas 200, 300, 400, 500, and 700 in this design) and are considered part of the total direct cost (TDC). Beyond the ISBL operations, the other process areas are considered outside battery limits (OSBL), including Areas 100 (rolled up into feedstock costs), 600, 800, and 900. Because TDC includes escalation factors only based on ISBL areas (see Table 30), the TDC is more inflated here relative to prior designs given the addition of the lignin-to-coproduct train (now Area 700), which is considered as additional ISBL operations, while Area 800 (lignin combustion/CHP) is considered as OSBL supporting operations.

Project contingency, field expenses, home office engineering and construction activities, and other costs related to construction are computed relative to the TDC and give the fixed capital investment (FCI) when summed. The sum of FCI and the working capital for the project is the TCI. Table 30 summarizes these categories and additional factors. The values assumed for each respective factor were maintained consistently with those discussed in the 2011 ethanol report [2] as well as the 2013 biological hydrocarbon report [10].

Table 30. Additional Costs for Determining TCI

Item	Description	Amount
Additional direct costs		
Warehouse	On-site storage of equipment and supplies.	4% of ISBL ^a
Site development	Includes fencing, curbing, parking lot, roads, well drainage, rail system, soil borings, and general paving. This factor allows for minimum site development assuming a clear site with no unusual problems such as right-of-way, difficult land clearing, or unusual environmental problems.	9% of ISBL
Additional piping	To connect ISBL equipment to storage and utilities outside battery limits.	4.5% of ISBL
Indirect costs		
Prorateable costs	This includes fringe benefits, burdens, and insurance of the construction contractor.	10% of TDC
Field expenses	Consumables, small tool and equipment rental, field services, temporary construction facilities, and field construction supervision.	10% of TDC
Home office and construction	Engineering plus incidentals, purchasing, and construction.	20% of TDC
Project contingency	Extra cash on hand for unforeseen issues during construction.	10% of TDC
Other costs	Includes: start-up and commissioning costs; land, rights-of-way, permits, surveys, and fees; piling, soil compaction/dewatering, and unusual foundations; sales, use, and other taxes; freight, insurance in transit, and import duties on items such as equipment, piping, steel, and instrumentation; overtime pay during construction; field insurance; project team; and parameters such as transportation equipment, bulk shipping containers, and plant vehicles.	10% of TDC

^a ISBL = installed cost of equipment inside battery limits (A200, 300, 400, 500, and 700).

Table 31. Project Cost Worksheet Including TDC and TCI (2016\$)

Process Area	BDO Pathway		Acids Pathway	
	Purchased Cost	Installed Cost	Purchased Cost	Installed Cost
Area 100: Feedstock Storage and Handling ^a	Included in feedstock cost		Included in feedstock cost	
Area 200: Pretreatment	\$35,800,000	\$48,700,000	\$35,800,000	\$48,700,000
Area 300: Enzymatic Hydrolysis and Hydrolysate Conditioning	\$9,100,000	\$15,400,000	\$31,100,000	\$62,700,000
Area 400: Enzyme Production	\$6,700,000	\$11,500,000	\$6,700,000	\$11,500,000
Area 500: Fermentation, Catalytic Conversion, and Upgrading	\$34,800,000	\$61,100,000	\$24,300,000	\$43,800,000
Area 600: Wastewater Treatment ^b	\$19,000,000	\$35,600,000	\$21,000,000	\$38,800,000
Area 700: Lignin Upgrading	\$60,800,000	\$128,400,000	\$60,300,000	\$127,500,000
Area 800: Combustor, Boiler, and Turbogenerator	\$28,200,000	\$51,000,000	\$26,900,000	\$48,700,000
Area 900: Utilities	\$9,000,000	\$15,500,000	\$9,900,000	\$17,200,000
Totals (Excl. Area 100)	\$203,500,000	\$367,200,000	\$217,000,000	\$398,900,000
Warehouse	4.0% of ISBL	\$10,600,000		\$11,800,000
Site Development	9.0% of ISBL	\$23,900,000		\$26,500,000
Additional Piping	4.5% of ISBL	\$11,900,000		\$13,200,000
Total Direct Costs (TDC)		\$413,600,000		\$450,400,000
Prorateable Expenses	10.0% of TDC	\$41,400,000		\$45,000,000
Field Expenses	10.0% of TDC	\$41,400,000		\$45,000,000
Home Office and Construction Fee	20.0% of TDC	\$82,700,000		\$90,100,000
Project Contingency	10.0% of TDC	\$41,400,000		\$45,000,000
Other Costs (Start-Up, Permits, etc.)	10.0% of TDC	\$41,400,000		\$45,000,000
Total Indirect Costs		\$248,200,000		\$270,200,000
Fixed Capital Investment (FCI)		\$661,800,000		\$720,600,000
Land		\$1,800,000		\$1,800,000
Working Capital	5.0% of FCI	\$33,100,000		\$36,000,000
Total Capital Investment (TCI)		\$696,800,000		\$758,400,000
Lang Factor (TCI/Purchased Equip Cost)		3.8		3.9
TCI per Annual Gallon Gasoline Equivalent		\$22.27/GGE		\$23.35/GGE

^a Feedstock handling not included in this calculation.

^b Area 600 not included in Lang factor.

4.3 Variable Operating Costs

Variable operating costs, which include raw materials, waste handling charges, and byproduct credits, are incurred only when the process is operating. Quantities of raw materials used and wastes produced were determined using the Aspen material balance. Table 32 documents the costs and sources of chemicals used in the process and Table 33 summarizes the variable costs on a per-year and per-GGE basis. The cost basis for most material costs in the present model that were also used in previous 2013 or 2011 design case models were left unchanged, aside from indexing to 2016\$. However, larger-cost items were revisited based on the most recent information available, including ammonia, sulfuric acid, glucose (concentrated glucose syrup), and diammonium phosphate, all updated based on averaging the most recent five-year cost history for each item (based on industry databases for all but glucose syrup, which was based on USDA sugar price data [149]). The cost of sodium hydroxide was also updated based on guidance from a recent subcontract with Nexant, set at \$0.23/lb in 2011\$, who also provided costs for sodium sulfate byproduct recovery equipment (discussed in Section 3.6) and resultant sodium

sulfate salt selling price, set at \$0.07/lb in 2011\$. As noted previously, the decision was made in this design to sell sodium sulfate salt after further purification of the WWT brine stream, given the substantial use of caustic and acid throughout the facility (i.e. during DMR pretreatment, lignin BCD, and muconic acid fermentation and recovery), which incurs significant costs equating to over \$1.30/GGE MFSP penalties for either fuel pathway, and would add another \$0.30/GGE for disposal (landfilling) of the waste brine. As this is untenable for ultimately achieving \$2.50/GGE MFSP targets, a portion of those costs are offset by selling the sodium sulfate byproduct.

Both pathways require a net power import after considering the amount of power generated through the CHP system, costed consistently with prior design cases with grid imports at 6.8 ¢/KWh (still reflective of current retail prices for the industrial sector as published by the Energy Information Administration [150]). Given a considerably larger usage of acids and bases in the present design, the cost for solids disposal (boiler ash and salt from WWT) is increased, with both ash and salt disposed to landfilling. Where needed, hydrogen was assumed here to be purchased as a product from standard natural gas-derived steam methane reforming (SMR) consistent with the 2013 report which utilized hydrogen for hydrotreating fatty acids. Net makeup hydrogen demands were calculated after including hydrogen co-produced and purified from both pathways' anaerobic fermentation steps; in the acids case, this translated to more hydrogen produced than required with the excess sent to the boiler, while the BDO case required additional net hydrogen import. The purchased hydrogen price was set based on a recent DOE Hydrogen and Fuel Cells Program report, which presented a current price for natural gas-based SMR hydrogen of \$1.57/kg (assumed in 2012\$) associated with a natural gas price of \$4/MM BTU [151], which was applied consistently following the 2013 biological hydrocarbon report. As this represents an SMR plant-gate price, this implies that the hydrogen plant is assumed to be co-located nearby with minimal costs for transportation "over the fence" to the biorefinery.

Adipic acid is co-produced in this design at a product purity over 99.7 wt%, with a sale price set at \$1,710/short ton (\$0.86/lb) in 2016\$. This aligns with purity requirements of 99.8% for production of nylon-6,6 via adipic acid as outlined in Vardon et al. [122]. Estimating prices for commodity chemicals is challenging as these prices vary on a quarterly, if not daily, basis. The cause for price variability is product specific and the reasons for these fluctuations range from impacts of feedstock costs to shifts in supply/demand, to unplanned outages at production facilities, to name a few common examples. Given the large impact that this coproduct price has on the underlying MFSP, this analysis strives to avoid any bias in the underlying assumption on commodity price cycles by a) utilizing a price reflective of the average value over the largest amount of data we have available, with the \$1,710/ton value attributed to a 15-year price average, and b) employing sensitivity analysis to evaluate the impact of the assumed price on the underlying MFSP. At the time of developing this write-up, the latest reported price of adipic acid in 2017 (US Gulf Coast) was roughly \$1,300/ton. Shifting the chemical price from \$1,710 to \$1,300/ton would increase the MFSP by over \$1/GGE. However, between the period of 2011 to 2015, the price of adipic acid fluctuated between \$2,300/ton and \$960/ton, in part reflecting trends in petroleum prices. Given this typical correlation between commodity chemicals and petroleum prices, it bears noting that relative to that same 2017 reference point at \$50/barrel oil, crude prices are projected by the U.S. Energy Information Administration to rise by 80% by 2030 (the target year tied to the *n*th-plant \$2.50/GGE MFSP goal for the facility to begin construction), or more than double by 2050 (year 20 of the subsequent 30-year facility lifetime), thus tempering possible concerns about the \$1,710/ton adipic acid price basis being optimistic over the plant lifetime relative to current market prices today.

Table 32. Chemical Costs and Sources

Component	Cost (2016\$)	Source
Biomass delivered to reactor throat	\$0.0285/lb	INL inputs, \$71.26/dry ton @ 20% moisture
Sulfuric acid, 93%	\$0.0430/lb	Industry database, 5-year average
Ammonia	\$0.1900/lb	Industry database, 5-year average
Sodium hydroxide	\$0.2384/lb	Nexant (indexed from 2011\$ basis)
Ultrafilter replacement	0.0297 \$/\$ cost	Nexant (annual cost per \$ membrane capex)
Corn steep liquor	\$0.0339/lb	Corn Products via Harris Group
Diammonium phosphate	\$0.1645/lb	Industry database, 5-year average
Corn oil (antifoam)	\$0.6439/lb	Industry database
Glucose	\$0.3670/lb	USDA ERS, 5-year average [149]
SO ₂	\$0.1811/lb	Industry database
Enzyme nutrients	\$0.4896/lb	Industry database (See 2011 design report for details)
Hydrogen	\$0.7306/lb	DOE report, SMR H2 @ \$4/MM BTU NG [151]
Hot oil system (utility heating)	\$5/MM BTU	Driven by NG prices
Toluene solvent (acids case)	\$0.3303/lb	Industry database
Ketonization catalyst (acids case)	\$2.95/lb	NREL internal database
Condensation catalyst (acids case)	\$9.07/lb	NREL internal database
HDO catalyst (acids case)	\$651/lb	NREL internal database
BDO upgrading catalyst (BDO case)	\$70/lb	NREL internal database
Oligomerization catalyst (BDO case)	\$70/lb	NREL internal database
HDO catalyst (BDO case)	\$528/lb	NREL internal database
Polymer for WWT	\$2.6282/lb	Brown and Caldwell 2012 WWT design [152]
Ethanol	\$0.3370/lb	Prior NREL analysis
Natural gas	\$5/MM BTU	Basis approximating historical NG prices
Lime	\$0.1189/lb	Harris Group
Boiler chemicals	\$2.9772/lb	2002 Design Report [3]
Cooling tower chemicals	\$1.7842/lb	2002 Design Report [3]
Fresh water	\$0.0002/lb	Peters and Timmerhaus [153]
Sodium sulfate salt coproduct value	\$0.0706/lb	Nexant (indexed from 2011\$ basis)
Adipic acid coproduct value	\$0.8554/lb	Average price over a 15-year cycle

Table 33. Variable Operating Costs

Process Area	Stream Description	BDO Usage (kg/hr) ^a	Acids Usage (kg/hr) ^a	BDO MM\$/yr (2016\$)	Acids MM\$/yr (2016\$)	BDO ¢/GGE (2016\$)	Acids ¢/GGE (2016\$)
Raw Materials							
N/A	Feedstock	104,167	104,167	51.62	51.62	164.94	158.94
A200	Sulfuric Acid, 93%	0	0	0	0	0	0
	Caustic (as pure)	5,833	5,833	24.17	24.17	77.25	74.44
	Ammonia	0	0	0	0	0	0
A300	CEH Filter Replacement	NA	Cost	NA	0.55	NA	1.69
A400	Glucose	1,324	1,324	8.45	8.45	26.99	26.01
	Corn Steep Liquor	90	90	0.05	0.05	0.17	0.16
	Corn Oil	7	7	0.08	0.08	0.26	0.25
	Ammonia	63	63	0.21	0.21	0.66	0.64
	Host Nutrients	37	37	0.31	0.31	1.00	0.97
	Sulfur Dioxide	9	9	0.03	0.03	0.09	0.09
A500	Corn Steep Liquor	608	1,308	0.36	0.77	1.14	2.37
	Diammonium Phosphate	71	190	0.20	0.54	0.65	1.67
	Hydrogen	410	0	5.21	0	16.66	0
	Hot Oil System (MM BTU/hr)	NA	37	NA	1.56	NA	4.80
	Toluene Solvent	NA	90	NA	0.52	NA	1.59
	Step 1 Catalyst ^b	1	0.2	0.62	0.01	1.97	0
	Step 2 Catalyst ^b	1	5,442	1.10	0.21	3.51	0
	Hydrotreating Catalyst ^b	0.2	0.3	0.24	0.46	0.77	0.01
A600	Ammonia	36	0	0.12	0	0.38	0
	Polymer	2	0	0.07	0	0.24	0
A700	Caustic (as pure)	2,660	2,401	11.03	9.95	35.23	30.64
	Ammonia	86	81	0.28	0.27	0.91	0.82
	Diammonium Phosphate	555	524	1.59	1.50	5.07	4.61
	Corn Steep Liquor	102	80	0.06	0.05	0.19	0.15
	Sulfuric Acid, 93%	10,835	10,531	8.10	7.87	25.88	24.24
	Ultrafilter Replacement	Cost	Cost	0.14	0.14	0.44	0.42
	Ethanol	37	37	0.22	0.21	0.70	0.66
	Hydrogen	406	0	5.16	0	16.48	0
A800	Boiler Chemicals	0.2	0.2	0.01	0.01	0.03	0.03
	FGD Lime (SOx control)	103	97	0.21	0.20	0.68	0.62
	Ammonia (NOx control)	1,054	1,215	3.48	4.01	11.12	12.35
	Natural Gas	1,300	0	2.68	0	8.56	0
A900	Cooling Tower Chemicals	2	3	0.06	0.10	0.21	0.32
	Makeup Water	133,396	209,901	0.36	0.56	1.14	1.73
Power	Grid Electricity (KW)	41,546	44,011	22.34	23.66	71.38	72.87
	Subtotal			146.60	137.40	468.47	423.08
Waste Disposal							
A800	Disposal of Ash	4,279	4,270	1.41	1.41	4.51	4.33
	Subtotal			1.41	1.41	4.51	4.33
Co-Products and Credits							
A600	Sodium Sulfate (98.5 wt%)	14,163	13,871	17.39	17.03	55.57	52.45
A700	Adipic Acid (99.7 wt% pure)	11,092	10,770	164.94	160.15	527.08	493.12
	Subtotal			182.33	177.18	582.65	545.57
Total Variable Operating Costs				-34.32	-38.37	-109.67	-118.15

^a For reference to convert to kg/GGE basis, fuel outputs are 3,969 and 4,119 GGE/hr for BDO and acids cases respectively.

^b Catalyst usage amortized to kg/hr-basis for consistency with rest of table. Step 1 = BDO upgrading (BDO), ketonization (acids); Step 2 = oligomerization (BDO), condensation (acids); Hydrotreating = hydrogenation (BDO), HDO (acids).

4.4 Fixed Operating Costs

Fixed operating costs are generally incurred in full whether or not the plant is producing at full capacity. These costs include labor and various overhead items. The assumptions on fixed operating costs were generally maintained consistently with the 2011 design basis (after updating to 2016\$ as described in Section 4.1), which in turn were based in large part on NREL’s 2002 ethanol design report [3] and/or Peters, Timmerhaus, and West [153].

Table 34 shows the recommended number of employees and associated salaries. The number of employees was estimated by considering the likely degree of automation for each area and adding a reasonable number of management and support employees. Details behind the originally assumed number of employees and associated salaries are provided in the 2011 ethanol report. Relative to that basis, some positions were expanded in light of the increased complexity and capital equipment expenditures reflected in the present design; namely plant engineers (4 rather than 2) and shift operators (24 rather than 20). Because the model feedstock is predominately corn stover, salaries were estimated for rural regions of the U.S. Midwest. These estimates may vary depending on location. While beyond the scope of this analysis, some economy-of-scale advantages could be gained with respect to labor costs by considering multiple units at the same site rather than a single stand-alone unit, such that some overlapping positions could be shared (e.g., one shared plant manager). However, such savings would likely be marginal in comparison to overall facility costs.

Table 34. Fixed Operating Costs

Position	2016 Salary	# Required	2016 Cost	MM\$/yr (2016\$)	BDO ¢/GGE (2016\$)	Acids ¢/GGE (2016\$)
Labor and supervision						
Plant Manager	164,452	1	164,452			
Plant Engineer	78,310	4	313,241			
Maintenance Supervisor	63,767	1	63,767			
Maintenance Technician	44,749	12	536,985			
Lab Manager	62,648	1	62,648			
Lab Tech	44,749	2	89,498			
Lab Tech-Enzyme	44,749	2	89,498			
Shift Supervisor	53,699	4	214,794			
Shift Operators	44,749	24	1,073,970			
Shift Operators-Enzyme	44,749	8	357,990			
Yard Employees	31,324	4	125,297			
Clerks and Secretaries	40,274	3	120,822			
Total Salaries			\$3,212,962	3.21	10.27	9.89
Labor Burden (90%)			\$2,891,655	2.89	9.24	8.90
Other Overhead			BDO MM\$/yr	Acids MM\$/yr	BDO Cent/GGE	Acids Cent/GGE
Maintenance	3.0% of ISBL		7.95	8.82	25.42	27.17
Property Insurance	0.7% of FCI		4.63	5.04	14.80	15.53
Total Fixed Operating Costs			18.69	19.97	59.73	61.50

A 90% labor burden is applied to the salary total and covers items such as safety, general engineering, general plant maintenance, payroll overhead (including benefits), plant security, janitorial and similar services, phone, light, heat, and plant communications. The 90% estimate is the median of the general overhead range suggested in the 2008 Process Economics Program Yearbook produced by SRI Consulting [154]. Annual maintenance materials were estimated as 3% of the installed ISBL capital cost and property insurance, and local property tax was estimated as 0.7% of the fixed capital investment, based on the 1994 Chem Systems report described in NREL's 2011 ethanol report. These factors are all consistent with those used in the 2011 and 2013 design reports.

4.5 Discounted Cash Flow Analysis and the Minimum Fuel Selling Price

4.5.1 Discount Rate

For this analysis, the discount rate (which is also the IRR in this analysis) was set to 10% and the plant lifetime was set to 30 years. The discount rate was also used in previous design reports and was based on the recommendation in Short et al. [155] on how to perform economic evaluations of renewable energy technologies for DOE. His view was that, "In the absence of statistical data on discount rates used by industrial, transportation and commercial investors for investments with risks similar to those of conservation and renewable energy investments, it is recommended that an after tax discount rate of 10%...be used." The 10% rate is consistent with all platforms across the BETO portfolio.

4.5.2 Equity Financing

Consistent with other recent design reports, it was assumed that the plant would be 40% equity financed. The terms of the loan were established at 8% interest for 10 years. The principal is taken out in stages over the 3-year construction period. Interest on the loan is paid during this period, but principal is not paid back (this is another n^{th} -plant assumption, which says that this cash flow comes from the parent company until the plant starts up). This is all consistent with the assumptions used in the 2013 biological hydrocarbon and the 2011 ethanol reports. Figure 19 illustrates the sensitivity of MFSP to the percentage of equity financing and the after-tax discount rate (the IRR).

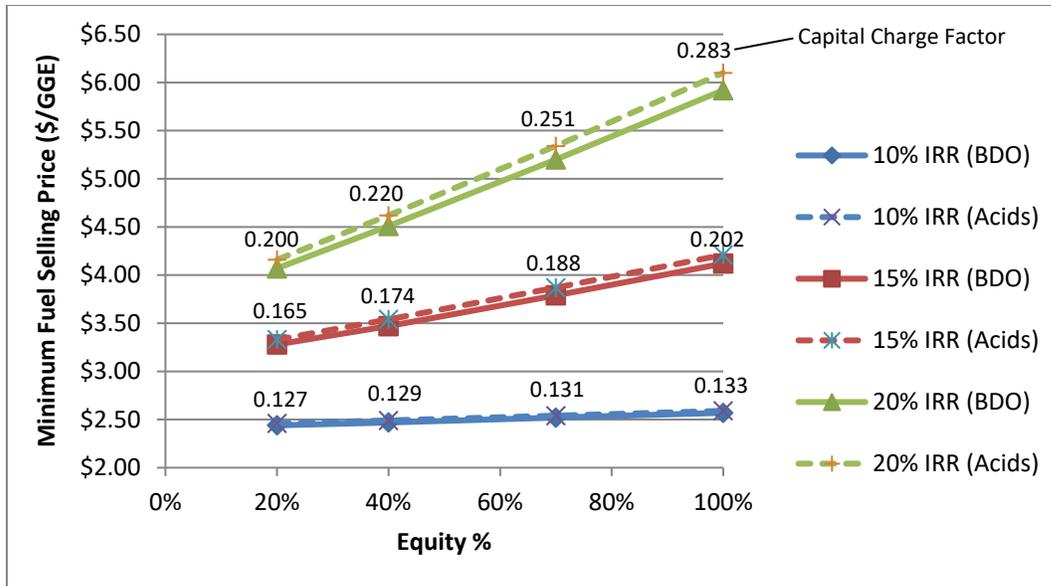


Figure 19. Sensitivity of MFSP to IRR and % equity for both fuel pathways. (8% interest on a 10-year loan.) Text labels over curves indicate corresponding capital charge factor (similar for BDO and acids cases).

4.5.3 Other Financial Metrics

Consistent with prior design cases, the IRS Modified Accelerated Cost Recovery System (MACRS) basis for depreciation schedules is maintained in the present design, which uses a 7-year recovery period for the majority of the plant except for the steam plant equipment (Area 800), which uses a 20-year recovery period. More details on depreciation considerations may be found in the 2011 design report. Next, the federal corporate tax rate used in the present analysis has been reduced from 35% (used in prior design cases) to 21%, reflective of recently passed tax legislation in December 2017 for permanent corporate tax rates. The amount of income tax to be paid by a potential fuel producer varies annually due to changes in the volume of product produced and the allowable depreciation deduction. In fact, no income tax is paid in the first 9 years of operation because the depreciation and loan interest deductions are greater than the net income. State taxes are not considered, primarily because the location of the plant has not been determined and tax rates vary from state to state (from 0% to 12%).

The construction time is important to the cash flow analysis because no income is earned during construction, but large sums of money are being expended. Construction time assumptions were left unchanged from the 2011 and 2013 design basis assumptions. Perry and Green [45] indicate that small projects (less than \$10 million investment) can be constructed in fewer than 18 months and that larger projects can take up to 42 months. An overview of petroleum refining economics indicates that large refineries (on the order of \$1.5 billion investment) can be constructed in 24 months [156]. Certainly, this facility is much smaller than a petroleum refinery, so using a construction time of 24 months fits within these references, although an important difference between this type of facility and a refinery is the large number of field-erected vessels. These are constructed on-site and have a longer construction time than if the tanks were delivered finished. Table 35 summarizes the schedule for construction and the cash flow during that time. Twelve months are added before construction for planning and engineering.

Table 35. Construction Activities and Cash Flow

Project Start Month	Project End Month	Activity Description	% of Project Cost
0	12	Project plan and schedule established; conceptual and basic design engineering and permitting completed; major equipment bid packages issued; engineering started on selected sub-packages; P&IDs complete; and preliminary plant and equipment arrangements complete.	8%
12	24	All detailed engineering—including foundations, structure, piping, electrical, and site—complete; all equipment and instrument components purchased and delivered; all site grading, drainage, sewers, rail, fire pond, foundation, and major structural installation complete; 80% of all major process equipment set (all except longest-lead items), all field fabricated tanks built; and the majority of piping and electrical materials procured.	60%
24	36	Complete process equipment setting, piping, and instrumentation installation complete; all electrical wiring complete; all building finishing and plumbing complete; all landscaping complete; pre-commissioning complete; and commissioning, start-up, and initial performance test complete.	32%
TOTAL			100%

Note: The above assumes no utility or process equipment orders placed prior to month seven. Expenditures are based on a typical 60 MM gal/yr grain-to-ethanol facility.

Similar to 2013 design basis, a start-up time of 6 months under an n^{th} -plant assumption was assumed in this analysis. Perry and Green [45] indicate that for a moderately complex plant, startup should be about 25% of the construction time, or 6 months in this case. The start-up period is not completely wasted, however. We expect that an average of 50% production could be achieved during that period while incurring 75% of variable expenses and 100% of fixed expenses. Finally, the present analysis applies the same basis for working capital as was used in the 2011 ethanol report, namely 5% of FCI. Peters, Timmerhaus, and West [153] define working capital as money available to cover (a) raw materials and supplies in inventory, (b) finished product in storage, (c) accounts receivable, (d) cash on hand for monthly payments such as wages and maintenance supplies, (e) accounts payable, and (f) taxes payable.

4.5.4 Base Case TEA Results

Table 36 summarizes the parameters used in the discounted cash flow analysis. Using these parameters, plus the cost information in Table 31, Table 33, and Table 34, the resulting MFSP of total fuel products is **\$2.47/GGE for the BDO case and \$2.49/GGE for the acids case (2016\$)**, including all fuel-range product cuts from distillation adjusted by heating values (calculated in the Aspen model) to gasoline equivalents.

Table 37 summarizes the yields and conversion costs for the present designs. According to the methodology of Cran [17], the expected accuracy of the overall TCI analysis is $\pm 25\%$ (although some specific pieces of equipment carry a higher degree of uncertainty in underlying cost estimates as identified above). If we apply this uncertainty to the TCI, the impact on the cost of total fuel is $\pm \$0.73/\text{GGE}$ and $\$0.77/\text{GGE}$ for the BDO and acids cases, respectively. The complete discounted cash flow summary worksheets are shown in Appendix B. The MFSP can be further broken down into the

cost of each process area. Figure 20 and Figure 21 illustrate the contribution to the overall cost by process area and capital, operations, and fixed costs (the bar for feedstock plus handling reflects the single feedstock cost of \$71.26/dry U.S. tons delivered to pretreatment and has not been broken down).

Table 36. Discounted Cash Flow Analysis Parameters

Plant life	30 years
Discount rate	10%
General plant depreciation	200% declining balance (DB)
General plant recovery period	7 years
Steam plant depreciation	150% DB
Steam plant recovery period	20 years
Federal tax rate	21%
Financing	40% equity
Loan terms	10-year loan at 8% APR
Construction period	3 years
First 12 months' expenditures	8%
Next 12 months' expenditures	60%
Last 12 months' expenditures	32%
Working capital	5% of fixed capital investment
Start-up time	6 months
Revenues during startup	50%
Variable costs incurred during startup	75%
Fixed costs incurred during startup	100%

Table 37. Summary of Yields, Rates, and Conversion Costs for Both Base Cases

	BDO Pathway	Acids Pathway
Feedstock rate	2,205 dry U.S. tons/day	
Online time	7,884 h/yr (90% online factor)	
Total fuel yield	43.2 GGE/dry U.S. ton feedstock	44.8 GGE/dry U.S. ton feedstock
Total fuel production rate	31.3 MM GGE/yr	32.5 MM GGE/yr
<i>Diesel-range production rate</i>	16.4 MM GGE/yr	32.5 MM GGE/yr
<i>Naphtha-range production rate</i>	14.9 MM GGE/yr	-
Adipic acid coproduct yield	266 lb/dry U.S. ton feedstock	259 lb/dry U.S. ton feedstock
Adipic acid production rate	193 MM lb/yr	187 MM lb/yr
Total variable opex excluding coproduct ^a	\$148 MM/yr	\$139 MM/yr
Coproduct revenue	\$182 MM/yr	\$177 MM/yr
Total fixed opex	\$19 MM/yr	\$20 MM/yr
Total equipment cost	\$367 MM	\$399 MM
Total capital investment (TCI)	\$697 MM	\$758 MM
TCI per annual gallon	\$22.27/GGE	\$23.35/GGE
Minimum Fuel Selling Price	\$2.47/GGE	\$2.49/GGE
Feedstock contribution	\$1.65/GGE	\$1.59/GGE
Fuel conversion contribution	\$3.83/GGE	\$3.87/GGE
Coproduct conversion contribution	-\$3.00/GGE	-\$2.97/GGE

^a Excludes coproduct revenue from sale of adipic acid and sodium sulfate (next row). Not including catalyst replacement schedules.

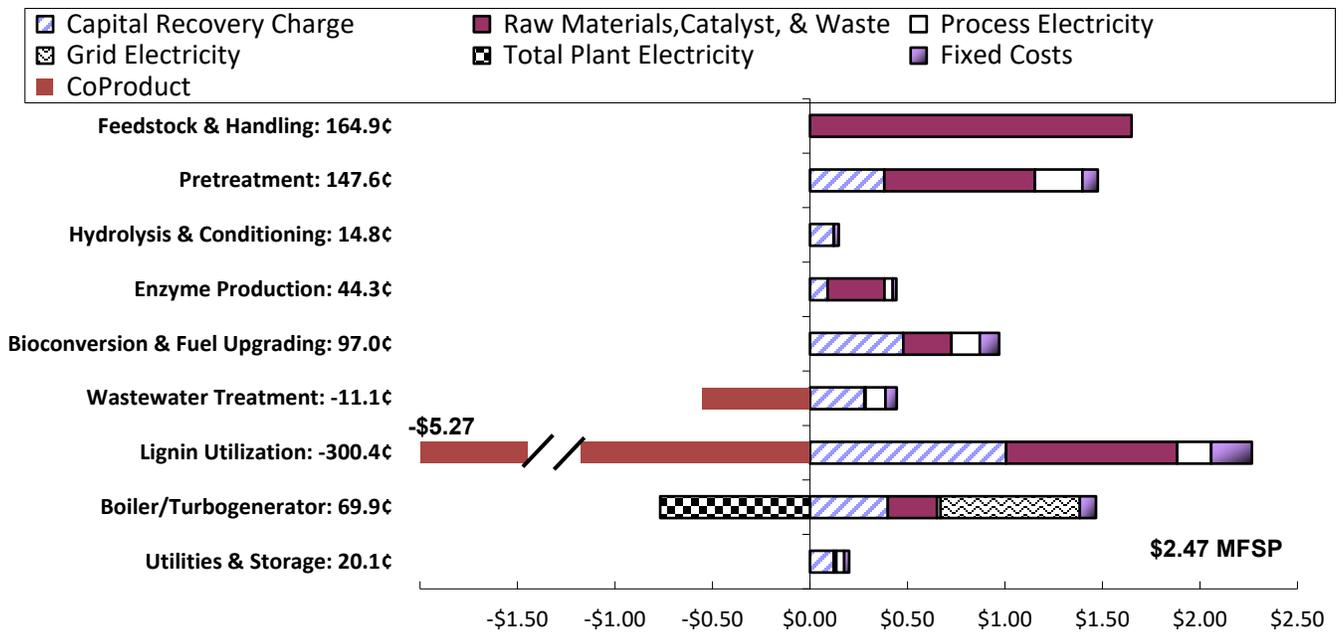


Figure 20. BDO pathway cost contribution details from each process area (per GGE total fuel products)

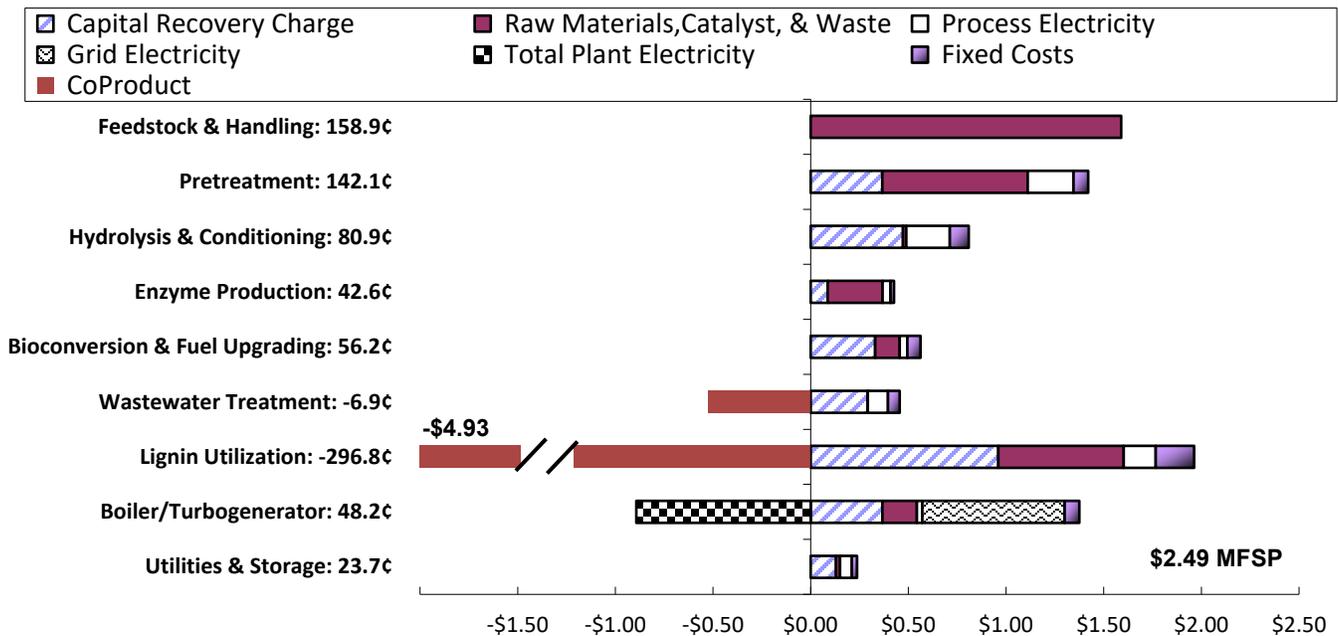


Figure 21. Acids pathway cost contribution details from each process area (per GGE total fuel products)

As shown in Table 37, Figure 20, and Figure 21, the MFSP estimates for both the BDO and acids pathways are seen to be quite comparable, with the BDO pathway exhibiting a roughly 3% lower yield (GGE/ton) but offset by a roughly 8% lower TCI. Variable operating costs for the BDO pathway are marginally higher than the acids pathway, primarily driven by a larger hydrogen deficit, due to catalytic upgrading demands versus hydrogen co-produced from fermentation. However, they are

counterbalanced by higher adipic acid coproduct yield/revenue, due to more unconverted sugars and other convertible components reaching the lignin train with the placement of solid separation downstream of BDO fermentation, and slightly lower fixed operating costs (partially tied to capital costs).

As is typical for TEA models, feedstock constitutes the largest MFSP contribution at roughly \$1.60–\$1.65/GGE, followed by pretreatment (DMR operations, including substantial costs for caustic demands) at nearly \$1.50/GGE and then either bioconversion and upgrading (BDO case) or hydrolysis and conditioning (acids case) at \$0.97/GGE and \$0.81/GGE for BDO and acids respectively. Also consistent with recent TEA models since 2013, enzyme contributions constitute one of the smaller cost drivers at the targeted 10 mg/g enzyme loading (this can be substantially higher at increased enzyme loading demands).

Comparing cost breakdowns in individual process areas, the acids pathway incurs a considerably larger cost for Area 300 (enzymatic hydrolysis and conditioning) on the order of \$0.66/GGE, due to more complex CEH processing than batch EH (although this includes the integrated solids removal steps which are required regardless for the acids pathway), as well as the inclusion of the hydrolysate evaporator. This is partially offset by lower costs for Area 500 (bioconversion and fuel upgrading) and 800 (CHP system). Area 500 costs contribute roughly \$0.41/GGE less for acids than BDO, primarily due to less costly catalytic upgrading steps designed to process only the acid intermediate (albeit at the added expense of pertraction membranes to first isolate the acid), versus the BDO pathway, which must process a much larger aqueous stream with roughly 90% water through the first BDO upgrading reactor. Indeed, the catalytic reaction steps taken in isolation are estimated to cost roughly \$36 MM for the BDO case versus \$21 MM for the acids case (installed equipment costs). Area 800 contributes roughly \$0.22/GGE less for acids than BDO, primarily due to lower biorefinery heat demands, which is driven in turn by catalytic upgrading that requires more heat for the BDO case given the much larger aqueous throughputs through the initial BDO upgrading step. Therefore, it is necessary to send more available steam through the turbine to generate more power. The differences between the other process area contributions generally reflect the fuel (GGE) and coproduct yield differences respectively. It is also worth noting that the wastewater treatment area now translates to a small net negative MFSP contribution after removing anaerobic digestion (typically the largest WWT cost driver) and including the sale of sodium sulfate coproduct.

5 Analysis and Discussion

5.1 Carbon, Water, and Energy Balances

Table 38 shows the overall flow of carbon inputs and outputs, with a carbon balance closure very near unity. As shown in the table, >96% of all carbon in the process enters in the biomass feed, with a small amount additional carbon primarily coming from glucose (for enzyme production) and natural gas (combusted in the boiler for supplemental heat in the BDO case). Bioconversion nutrients like CSL are a very minor contributor to the carbon balance. For the most part, fermentor vents are routed to the boiler in Area 800 and are reflected as flue gas. In both cases, roughly 40% of the carbon input leaves as fuels and coproducts, allocated roughly 65% to fuels and 35% to coproducts. The carbon yield to fuels at 24%–26% is similar (slightly lower) compared to prior biological pathway models i.e. the 2011 ethanol and 2013 hydrocarbon design reports at 29% and 26%, respectively, but with the addition of coproducts derived from lignin, extractives, and other residual carbon components adding another 14%, the resulting overall biorefinery carbon yield to “useful” products is now substantially improved. Major exit points for the balance of carbon are the combustor stack and the aerobic digestion lagoons.

Table 38. Biorefinery Overall Carbon Balance

Stream	Acids Case		BDO Case	
	Carbon Flow (kmol/h)	% of Carbon Flow	Carbon Flow (kmol/h)	% of Carbon Flow
Carbon inlets				
Biomass feedstock	3,084	97%	3,084	96%
Natural gas	-	-	81	2%
Glucose	44	1%	44	1%
Chemical inputs	40	1%	20	1%
Total	3,168	100%	3,230	100%
Carbon outlets				
Area 500 fuel output	808	26%	770	24%
Area 700 coproduct	443	14%	457	14%
Combustor flue gas	1,770	56%	1,796	56%
Aerobic lagoons	144	5%	214	7%
Total	3,164	100%	3,238	100%

The overall flow of water throughout the model is presented in Table 39 and Table 40. Cooling tower evaporation accounts for the majority of the total process makeup water demand. Between the two pathways, the BDO case translates to a lower process makeup water demand at 8.9 versus 13.5 gal/GGE (and lower overall water “input” of 13.6 versus 17.4 gal/GGE). This is due primarily to higher TS concentrations through enzymatic hydrolysis and fermentation (i.e., batch EH requires less dilution water than CEH). As discussed above, lower A800 excess steam availability and thus condensing steam turbine cooling demands in the BDO case also contribute to the differences in makeup water demand.

Table 39. Biorefinery Water Balance, Acids Case

Water Balance					
Inputs	kg/hr	gal/GGE	Outputs	kg/hr	gal/GGE
Moisture in feedstock	20,833	1.3	Cooling tower losses	195,823	12.6
Water in glucose syrup	234	0.0	Fermentor vents	424	0.0
Water in raw chemicals	1,627	0.1	WWT evaporation	21,968	1.4
Net reaction water	28,483	1.8	WWT discharge	158	0.0
Air intake moisture	9,611	0.6	Boiler blowdown vent	1,558	0.1
Makeup water	209,901	13.5	Flue gas	50,737	3.3
			Water in product	21	0.0
Sum of Inputs	270,689	17.4	Sum of Outputs	270,688	17.4

Table 40. Biorefinery Water Balance, BDO Case

Water Balance					
Inputs	kg/hr	gal/GGE	Outputs	kg/hr	gal/GGE
Moisture in feedstock	20,833	1.4	Cooling tower losses	121,177	8.1
Water in glucose syrup	234	0.0	Fermentor vents	424	0.0
Water in raw chemicals	1,308	0.1	WWT evaporation	22,096	1.5
Net reaction water	37,894	2.5	WWT brine	87	0.0
Air intake moisture	10,457	0.7	Boiler blowdown vent	1,950	0.1
Makeup water	133,396	8.9	Flue gas	58,324	3.9
Sum of Inputs	204,121	13.6	Sum of Outputs	243,000	13.6

Finally, Figure 22 presents energy balance allocations for all energy outputs embodied in each major exit point from the biorefinery. Energy in the fuel product, adipic acid coproduct, heat rejection to the cooling tower, and out the flue gas stack constitute the primary energy output flows. Energy outputs in all “useful” products (i.e. the fuel and coproduct combined) represent between 39-43% of total biorefinery outputs, while “waste” heat rejection from cooling water and air cooler utilities constitutes 30-33% across the two pathways. It is worth noting here that relative to prior biochemical design cases, the present design makes significantly more use of both biological (low-temperature) and catalytic (high-temperature) processing steps, given the catalytic upgrading train required for both pathways after sugar fermentation to fuel precursors, as well as elevated temperatures for lignin deconstruction and coproduct upgrading. While efforts were made to optimize process heat integration, further room for better optimization may still exist to reduce waste heat losses through more rigorous pinch analysis, as an area for further refinement moving forward. Even so, energy losses to “waste” outputs other than the primary products are always inevitable in any integrated process such as this.

It should also be noted that the overall energy flows are derived from inputs beyond just the biomass feed. Table 41 shows a high-level energy balance of all energy input and output flows. Biomass feedstock constitutes 349 MMkcal/hr, which represents 84% of all energy inputs for the acids case (416 MMkcal/hr total) or 78% of all inputs for the BDO case (449 MMkcal/hr total). Imported power, natural gas, and raw chemicals also carry considerable embodied energy input flows for both pathways. Total energy inputs are higher for the BDO pathway given more natural gas heating demands as well as a hydrogen deficit which requires importing additional hydrogen.

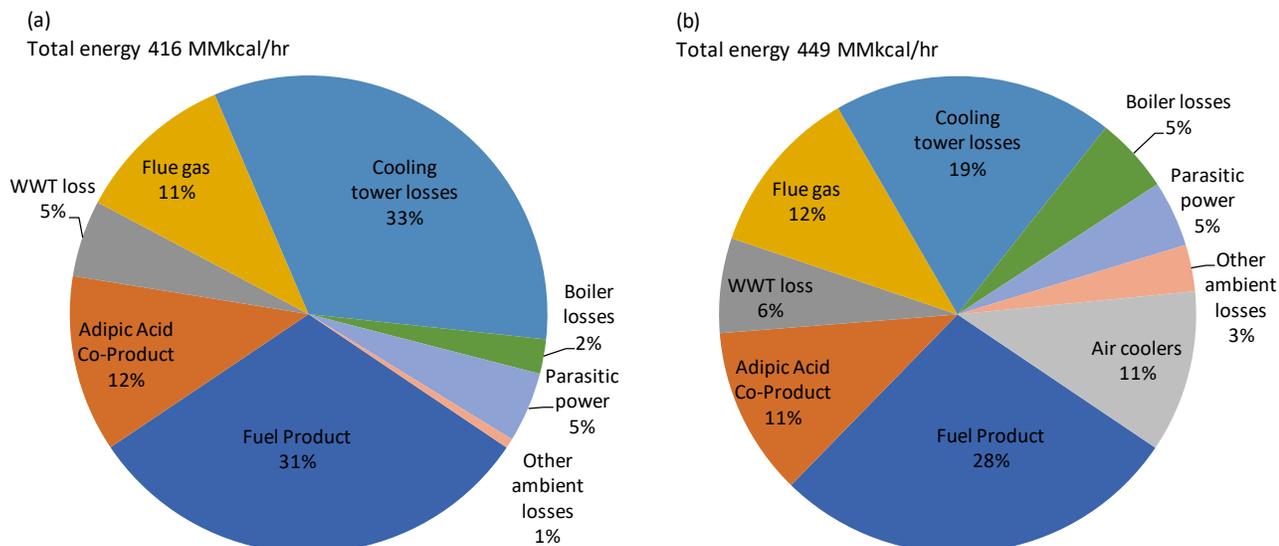


Figure 22. Distribution of energy outputs embodied in major exit points; (a) acids case, (b) BDO case

Table 41. Overall Input/Output Energy Balances

Inputs (MMkcal/hr)	Acids	BDO	Outputs (MMkcal/hr)	Acids	BDO
Feedstock	349	349	Fuel Product	130	125
Glucose Syrup	5	5	Adipic Acid Co-Product	50	51
Raw chemicals	12	8	WWT losses ^b	22	28
Fresh water ^a	-2	-1	Flue gas	45	51
Air	6	6	Cooling tower losses	138	85
Imported power	39	36	Boiler losses	10	23
Natural gas	8	17	Air Cooler	-	49
Hydrogen	0	28	Parasitic power	20	20
			Other ambient losses	3	14
Sum of Inputs	416	449	Sum of Outputs	416	449

^a Value appears negative due to selected reference states for calculating enthalpy flows.

^b Includes energy outputs in WWT brine plus aerobic lagoon evaporation

5.2 Cost Sensitivity Analysis

For each of the pathways described previously in the report, the techno-economic models were used to perform sensitivity analysis on key model variables. Beginning with the baseline for each variable as described in this report, minima and maxima were chosen based on reasonable limits surrounding the specific process, conversations with researchers, and expected error margins on capital costs. Each variable was changed to its maxima/minima with all other factors held constant. The resulting model outputs are used to help understand and quantify cost impacts on the overall MFSP.

5.2.1 Single-Point Sensitivity Analysis: Acids to Fuels Pathway

For the acids pathway, key parameters for pretreatment, hydrolysis, fermentation, and upgrading, as well as lignin utilization, were explored. Table 42 lists the studied variables, their baseline values, and the associated minima/maxima. The sensitivities of (a) MFSP and (b) fuel product yield are displayed as tornado charts in Figure 23. For the yield studies, not all variables showed a significant effect and only a subset of the metrics used in Table 42 are included in the tornado chart.

The uncertainty in capital cost associated with the factored approach used in this study ($\pm 25\%$ TCI) shows the largest impact on MFSP and is more pronounced compared to previous designs due to the increase in overall capital associated with an additional lignin processing train. Beyond capital costs, the amount of lignin accessible to the muconate fermentation (or viewed alternatively, the net overall conversion potential to muconic acid from original lignin in the delivered biomass inclusive of BCD deconstruction and bioconversion) and the muconic acid fermentation productivity have the next largest impacts on MFSP, i.e. lignin train conversion performance reflects the two largest single process-related sensitivity parameters. As a simplistic estimate for what might be required to achieve more near-term \$3/GGE MFSP goals by 2022 as an interim benchmark on the path to $< \$2.50/\text{GGE}$ by 2030, if all other target conversion parameters remained unchanged, overall conversion efficiency of biomass lignin to adipic acid could be relaxed by roughly 12% from 259 to 229 lb/dry ton, inclusive of lignin deconstruction and conversion yields. This is assuming that many other parameters could also be achieved by 2022, for example in the fuel train and downstream lignin upgrading steps. This is also inclusive of a higher interim 2022 biomass feedstock cost projection at \$79.07/dry ton (versus the final 2030 target cost of \$71.26/dry ton) based on inputs from INL, translating to an interim MFSP of \$3.02/GGE.

For the fuel train parameters, the butyric acid separation efficiency has the largest effect on fuel yield and a correspondingly large impact on MFSP. Following acid product recovery, the CEH solids loading also reflects a major MFSP impact, particularly if solids loading dropped from 7.5% to 5% given substantial costs for re-concentrating the clarified sugars. Net conversion of sugars to products during fermentation has a large effect on overall fuel yield which includes glucose, xylose, and arabinose contributions, but is also affected by the amount of contamination to non-acid products that occurs. We note here that operating parameters varied in the underlying process model have impacts on multiple economic contributors including product yield, capital costs, and operating costs, and more properly represent risks or alternatively represent a range of results that are possible depending on the operation and success of the bench- and pilot-scale campaigns. In comparison, varying a parameter like the TCI $\pm 25\%$ represents a true uncertainty surrounding the modeling methodology or price estimates.

Table 42. Assumptions Varied in the Acids Sensitivity Analysis

	Assumption	Min MFSP	Baseline	Max MFSP
Pretreatment	DMR NaOH loading (mg/g)	50	70	100
	DMR xylan to liquor (wt%)	25.0%	10.0%	5.0%
	DMR lignin to liquor (wt%)	60.0%	47.0%	25.0%
Continuous Enzymatic Hydrolysis	CEH cellulose to glucose (wt%)	99.0%	96.3%	90.0%
	CEH xylan to xylose (wt%)	99.0%	98.9%	90.0%
	CEH Solids loading (wt%)	10.0%	7.5%	5.0%
	CEH ultrafilter permeance	80	66.66	50
	CEH microfiltration permeance	115	99.99	85
	Flocculant Requirement (g/kg Solid)	-	0	20
Enzyme Production	Enzyme production capital cost	-50%	-	+50%
	Enzyme Licensing	-	0	0.1
Acid Fermentation and Catalysis	Fermentation contamination loss (wt%)	0%	3%	6%
	Fermentation glucose to product (wt%)	100%	95%	85%
	Fermentation xylose to product (wt%)	90%	85%	75%
	Fermentation arabinose to product (wt%)	90%	85%	75%
	Fermentation Productivity (g/L/hr)	2.5	2	1.5
	Fermentation bioreactor volume (gal)	-	1MM gal	0.2MM gal
	Pertraction butyric acid recovery (wt%)	-	1	0.85
	Condensation solvent:ketone ratio (w/w)	5	3.64	1
	Condensation single pass conversion	90%	60%	40%
	Fermentation pertraction membrane cost	-50%	-	150%
	Acid ketonization WHSV (hr-1)	10	6	2
	Condensation residence time (hr)	5	15	24
	Enone hydrogenation WHSV (hr-1)	10	3	1
	Enone hydrogenation Platinum loading (wt%)	1%	3%	-
Acid catalysis train capital cost	-50%	-	150%	
Lignin Utilization	Muconic metabolic yield (g/g sugar)	0.408	0.3076	-
	Muconic productivity (g/L/hr)	2	1	0.5
	Muconic acid fermentation pH control	none	controlled	-
	Muconic acid hydrogenation Temperature (°C)	100	78	-
	Sugar diversion to coproduct (wt% clean sugar)	10%	0%	-
	Metabolically accessible lignin (wt%)	0.675	0.5333	0.405
	Oslo Crystallizer capital cost	-20.0%	-	20.0%
Economics	Total capital investment (TCI)	-25.0%	-	25.0%
	Feedstock Cost (\$/dry ton)	60	71.26	80

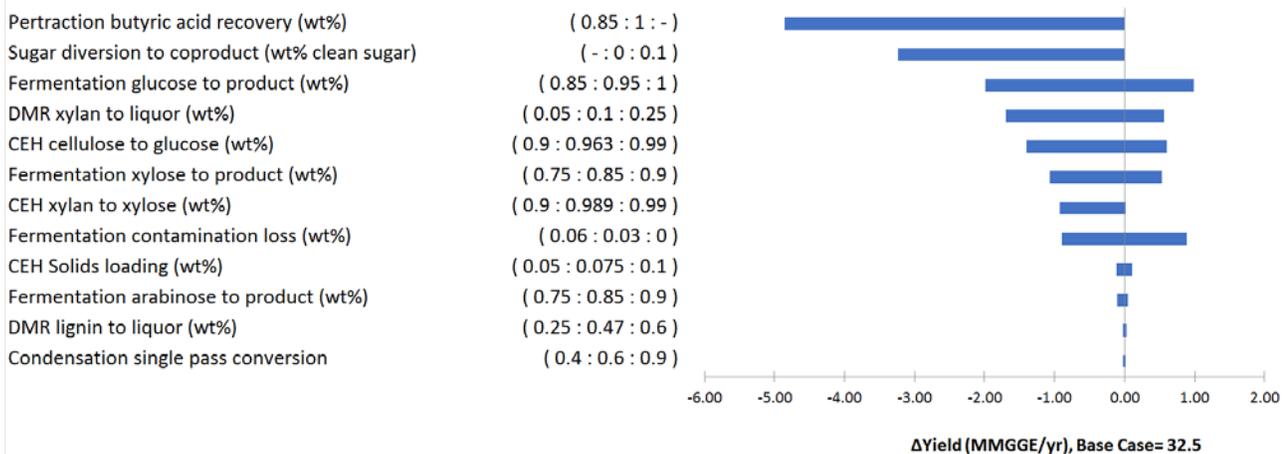
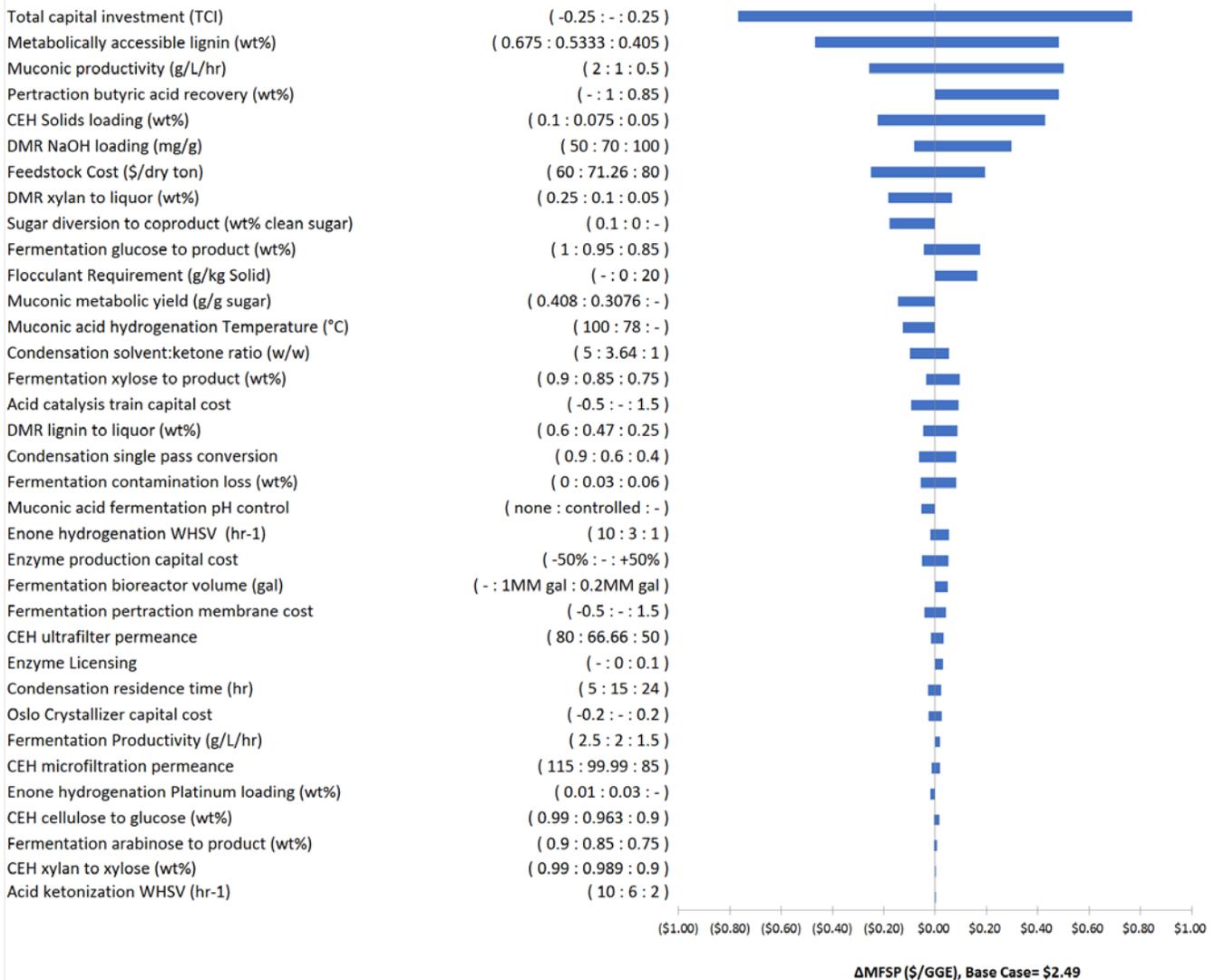


Figure 23. Acids single-point sensitivity tornado charts for MFSP and production yield

5.2.2 Single-Point Sensitivity Analysis: BDO to Fuels Pathway

As in the acids pathway, similar parameters for pretreatment, hydrolysis, fermentation, and upgrading, as well as lignin utilization, were explored for the BDO pathway. Table 43 lists the studied variables, their baseline values, and the associated minima/maxima. The sensitivities of (a) MFSP and (b) fuel product yield are displayed as tornado charts in Figure 24.

Similar to the acids pathway, the uncertainty in capital cost has the largest impact on MFSP and is more pronounced compared to previous designs due to the increase in overall capital associated with an additional lignin processing train, as well as a more complicated catalytic upgrading train. Beyond capital costs, the amount of lignin accessible to the muconate fermentation and the muconate fermentation productivity are again the next largest MFSP drivers. Also similar to the above acids case, for a more near-term interim goal of \$3/GGE by 2022, overall biomass lignin conversion to adipic acid could be relaxed by roughly 12%, from 266 to 235 lb/dry ton biomass (after also increasing the biomass feedstock cost to the 2022 interim target of \$79.07/dry ton as noted above) at a resulting MFSP of \$2.99/GGE.

For the fuel train via BDO, the largest cost drivers are enzyme loading, DMR caustic loading, and enzymatic hydrolysis solids content (primarily impacting the downstream BDO concentration and thus catalytic upgrading costs). The amount of cellulose hydrolyzed to glucose reflects the largest effect on fuel yield followed by the fermentation conversion of hydrolyzed glucose to product. Similarly but with a smaller magnitude, the net conversion of the minor sugars to products during hydrolysis and fermentation also has a substantial effect on overall fuel yield, which includes xylose and arabinose contributions, but is also affected by the amount of contamination to side product species. As above, the distinction between uncertainty in capital cost estimates and economic parameters compared to process/technical risks should be noted.

Table 43. Assumptions Varied in the BDO Sensitivity Analysis

	Assumption	Min MFSP	Baseline	Max MFSP
Pretreatment	DMR NaOH loading (mg/g)	50	70	100
	DMR xylan to liquor (wt%)	25%	10%	5%
	DMR lignin to liquor (wt%)	60%	47%	25%
Continuous Enzymatic Hydrolysis	EH Solids loading (wt%)	30%	25%	20%
	EH cellulose to glucose (wt%)	95%	90%	75%
	EH xylan to xylose (wt%)	95%	90%	75%
	EH enzyme loading mg/g	5	10	20
	EH time (d)	3.5	5	6
	Flocculant Requirement (g/kg solid)	-	0	20
Enzyme Production	Enzyme production capital cost	-50%	-	+50%
	Enzyme Licensing	-	0	0.1
BDO Fermentation and Catalysis	Fermentation contamination loss (wt%)	0%	3%	6%
	Fermentation glucose to product (wt%)	100%	95%	85%
	Fermentation xylose to product (wt%)	95%	90%	80%
	Fermentation arabinose to product (wt%)	95%	85%	75%
	Lignin press S/L capital cost	-50%	-	50%
	Microfilter retentate loss	0	0.01	0.03
	BDO upgrading WHSV	3	2	1
	Oligomerization reactor WHSV	3	1	0.5
	BDO catalysis capital cost	-50%	-	100%
	H2 price (\$/kg)	1	1.57	2
	BDO upgrading reaction temperature (°C)	150	250	-
	BDO upgrading catalyst cost	-50%	-	50%
	Oligomerization catalyst cost	-50%	-	50%
Lignin Utilization	Muconic metabolic yield (g/g glu)	0.408	0.3076	-
	Muconic productivity (g/L/hr)	2	1	0.5
	Muconic acid fermentation pH control	none	controlled	-
	Muconic acid hydrogenation Temperature (°C)	100	78	-
	Sugar diversion to coproduct (wt% clean sugar)	0.1	0	-
	Metabolically accessible lignin (wt%)	68%	53%	41%
	Oslo Crystallizer capital cost	-20%	-	20%
Economics	Total capital investment (TCI)	25%	-	-25%
	Feedstock Costs (\$/dry ton)	80	71.26	60

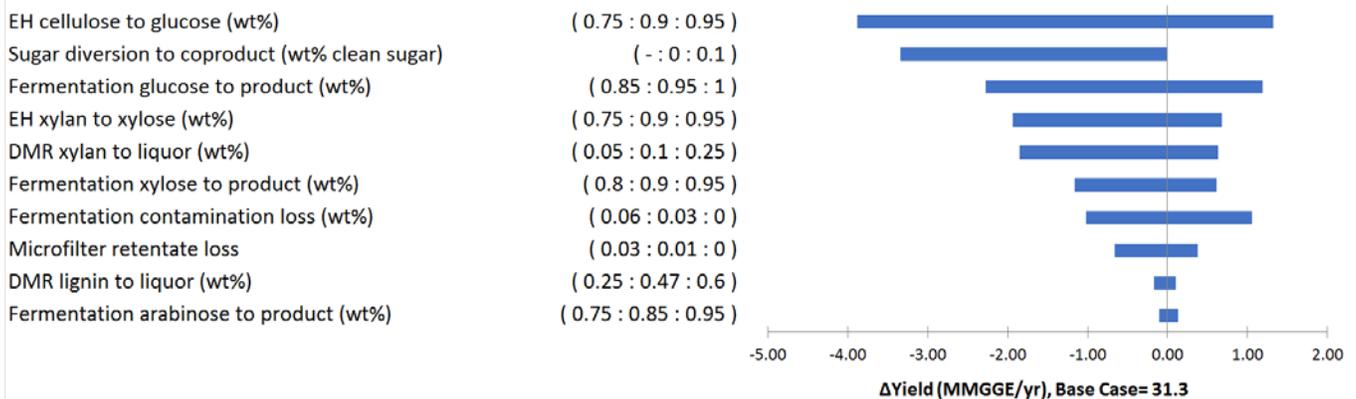
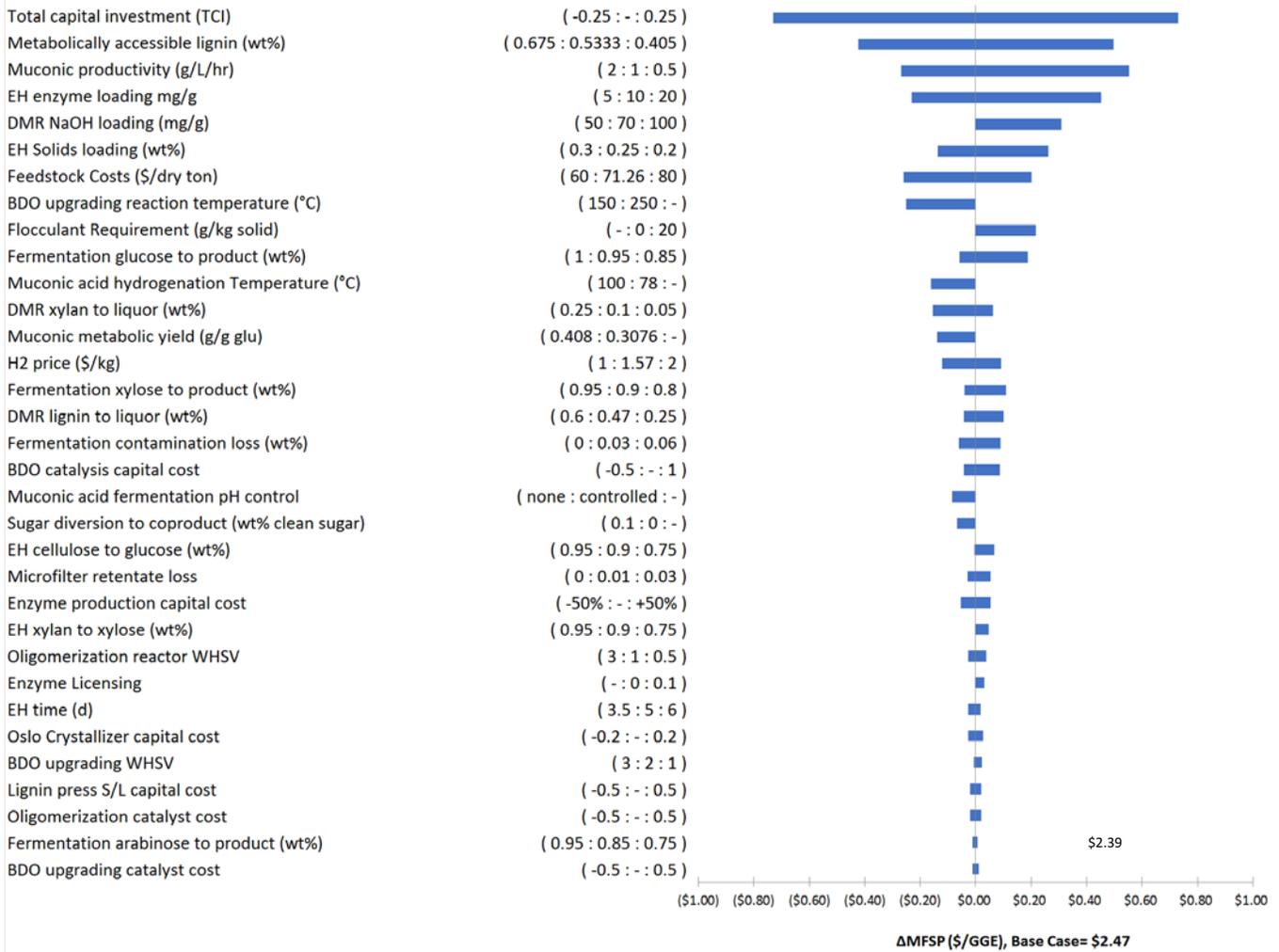


Figure 24. BDO single-point sensitivity tornado charts for MFSP and production yield

5.2.3 MFSP Sensitivity to Adipic Acid Co-Product Value

As noted above, the market value of adipic acid has fluctuated significantly over recent years, as is typical for many chemical products as a function of petroleum prices and market conditions. Given this dynamic, a 15-year average price was selected as the base case here, at \$0.86/lb (each year's nominal US Gulf Coast price was first inflated to 2016\$ and then averaged). To highlight the strong sensitivity this value exhibits on overall biorefinery economics, Figure 25 shows the MFSP implications for adipic acid market value ranging from \$0.5/lb (representing the lowest price point over that timeframe) up to \$1.25/lb (representing the point when MFSP would approach \$0/GGE, although the value has exceeded this range). Over that price range, the resulting MFSP for both the acids and BDO pathways varies substantially over a span of \$4.5/GGE, demonstrating that this parameter exhibits a very strong influence on overall biorefinery economics at the base case lignin conversion targets projected here. While this is not a new finding and is in line with prior TEA modeling for similar biorefinery concepts employing a high-value coproduct [157], it highlights the importance of understanding and anticipating market dynamics when planning to construct and operate a biorefinery of this nature, ideally exhibiting the capacity to respond to changing market conditions by producing different products or maximizing fuel versus product outputs. At the base case adipic acid yields projected in this design, the current global market for adipic acid (2.8 MM tonne/year) would be met with approximately 33 biorefineries of this size. However, as noted throughout this report, adipic acid is intended to represent *one example* of many other potential products from lignin (or sugars), and in reality different biorefineries would be expected to produce different products as prevailing market conditions dictate, just as petrochemical facilities do not all produce the same individual products.

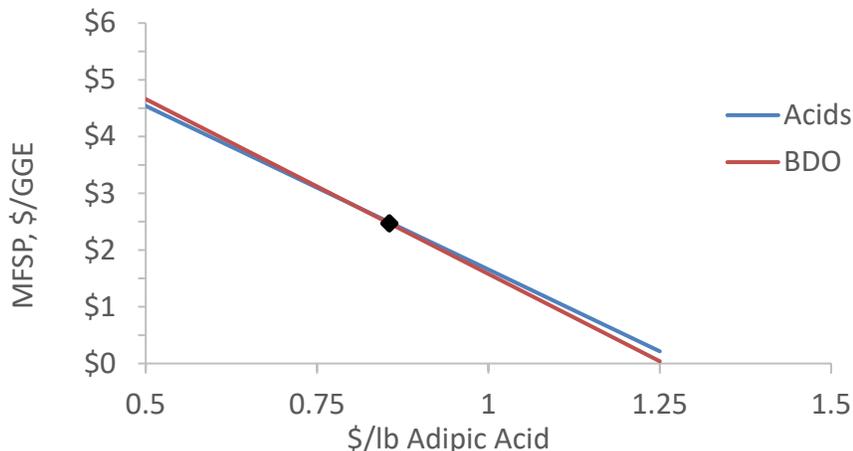


Figure 25. MFSP sensitivity to adipic acid selling price for both fuel train pathways. Marker indicates base case price assumed in this design (\$0.86/lb) based on 15-year adipic acid price history.

5.3 Sustainability Metric Indicators

This section presents primary sustainability metric indicators of the current conceptual process at the conversion stage. Direct CO₂, NO₂, and SO₂ emissions from the biorefinery, water consumption, and other process-related metrics were taken directly from the Aspen conversion process models described above. The material and energy flows of the conversion step capture the impacts of input raw materials, and outputs such as fuel yields, wastes, and coproducts as predicted by the process model, and are shown in Table 44.

The input/output inventories in Table 44 also provide the necessary information required for performing life cycle analysis (LCA) modeling to quantify greenhouse gas (GHG) emissions and fossil energy consumption. The biorefinery GHGs and fossil energy consumption will be calculated separately under supply chain sustainability analysis efforts coordinated by partners at Argonne National Laboratory in the future and are not reported here. A complete well-to-wheel or supply chain LCA evaluation is required to more fully understand the sustainability implications for the full supply chain based on this technology pathway, such as how the overall integrated biorefinery GHG emissions profiles compare to BETO goals relative to petroleum diesel. One key driver in the system LCA is the inclusion of a non-fuel coproduct (e.g., adipic acid and sodium sulfate). When produced in significant quantities, as is the case here, it can strongly influence the overall GHG emissions (with the potential for substantial GHG credits relative to energy-intensive synthesis of a material such as fossil-derived adipic acid), depending on the coproduct handling method selected for the LCA [158].

Table 45 summarizes the key sustainability metric indicators for the two conversion processes evaluated here. The fuel yield, carbon efficiency to fuels and chemical coproduct (e.g., adipic acid), as well as the electricity import are comparable for the two cases. The overall combined carbon efficiency (to fuel and adipic acid) for the acids pathway and BDO pathway are roughly 41% and 40%, respectively. The BDO pathway is more energy-intensive, particularly with respect to aqueous catalytic upgrading, and thus requires natural gas supplementation in the boiler (15.4 MJ/GGE). The acids pathway does not require natural gas supplementation in the boiler, but does use a separate natural gas-fired heater system for hot oil circulation in servicing high-temperature heating needs discussed previously (9.6 MJ/GGE). The acids pathway exhibits higher water consumption at the conversion stage, as discussed previously. On an energy basis, the water consumption for the acid and BDO pathways are 13.5 gal/GGE (5,041 m³/day) and 8.9 gal/GGE (3,203 m³/day), respectively. Biorefinery net water consumption includes, but is not limited to, water that is incorporated into the product and evaporation directly from process operations or indirectly from cooling and heating processes (e.g., cooling tower evaporative losses). The relatively high water demands for these processes may impose constraints on facility siting locations, requiring sufficient access to local water resources while also being located in areas suitable for meeting delivered feedstock compositional/cost targets discussed in Section 3.1.

Table 44. Input and Output Inventory Data Associated with the Modeled Conversion Facility

Pathways (via intermediates)	Acids	BDO
Products	Production Rate	Production Rate
Hydrocarbon Fuel	11,465 kg/hr	11,032 kg/hr
	504,671 MJ/hr (LHV)	486,293 MJ/hr (LHV)
Co-products		
Adipic Acid (Polymer Grade)	10,770 kg/hr	11,092 kg/hr
Recovered sodium sulfate salt from WWT	13,871 kg/hr	14,163 kg/hr
Export Electricity	0 kW	0 kW
Resource Consumption	Flow Rate (kg/hr)	Flow Rate (kg/hr)
Biomass Feedstock (20% moisture)	104,167	104,167
Sulfuric Acid, 93%	10,531	10,835
Caustic (as pure)	8,235	8,494
Ammonia	1,359	1,238
Glucose	1,324	1,324
Corn Steep Liquor	1,478	800
Corn oil	7.3	7.3
Host nutrients	37	37
Sulfur Dioxide	9.0	9.0
Diammonium Phosphate	714	627
Toluene Solvent Makeup	90	0
Hydrogen	0	816
Ethanol	37	37
Boiler Chemicals	0.2	0.2
FGD Lime	97	103
Cooling Tower Chemicals	3.4	2.1
Makeup Water	209,901	133,396
Natural Gas for Boiler	0	1,300
Natural Gas for Hot Oil System	37.3 MMBtu/hr	0
Grid Electricity (Net Import)	44,011 kW	41,546 kW
Waste Streams	Flow Rate (kg/hr)	Flow Rate (kg/hr)
Disposal of Ash	4,270	4,279
Air Emissions	Flow Rate (kg/hr)	Flow Rate (kg/hr)
H2O	55,465	62,998
N2	362,108	394,980
CO2 (biogenic)	82,513	83,456
CO2 (fossil)	2,225	3,575
O2	59,291	57,766
NO2	8.4	19.6
SO2	5.8	6.7
CO	42.2	53.9
CH4	0	0

Table 45. Summary of Sustainability Metric Indicators for the Modeled Biorefinery Process

Sustainability Metrics		Pathways (via intermediates)	
		Acids	BDO
Fuel Yield by Weight of Biomass	GGE per dry ton biomass	44.8	43.2
Carbon Efficiency to Fuels	% C in feedstock	26.2	25.0
Carbon Efficiency to Adipic Acid	% C in feedstock	14.4	14.8
Electricity Import	KWh/GGE	10.7	10.5
Natural Gas Import	MJ/GGE	9.6	15.4
Water Consumption	gal/GGE	13.5	8.9
Water Consumption	m ³ /day	5,041	3,203

5.4 Additional Opportunities for Cost Reduction

Beyond the process configurations considered here through rigorous TEA modeling, a number of additional opportunities exist to further reduce fuel costs and/or achieve similar cost targets through different approaches. While outside the scope of the present modeling work, these opportunities are briefly discussed on a high level below, and may be evaluated in more detail in the future.

Waste CO₂/Biogas Utilization

In this design, vented gas from sugar fermentation, lignin conversion, and boiler flue gas represent a substantial amount of wasted carbon as CO₂ (roughly 26,000 kg/hr, 10,000 kg/hr, and 78,000 kg/hr, respectively). The flue gas from the boiler is the main CO₂ stream taking up ~60% of the total CO₂ produced in the process. Conversion of waste CO₂ into transportation fuels and chemicals represents a significant opportunity for transforming abundant gaseous resources into a variety of materials and chemicals. However, even with this large potential, commercial expansion in this area has been limited due to the lack of information and understanding around the economic viability of the emerging CO₂ conversion technologies.

Highlighting only reductive pathways, four pathways stand out for CO₂ upgrading to chemicals and fuels: biochemical, thermochemical, electrochemical, and bioelectrochemical. A microbial-assisted CO₂ electrolyser is a promising option to integrate wastewater treatment and waste CO₂ utilization. Bioelectrochemical systems are shown to be more effective at treating wastewater that contains high concentrations of volatile fatty acids, such as wastewater produced by hydrolysis and fermentation. In the present design, the bioelectrolysis process has the potential to replace the aerobic digestion step, which followed anaerobic digestion in previous biochemical design models for future wastewater treatment. Depending on the configuration and routing of DMR liquor, acetate salts may reach wastewater treatment, which are very suitable for bioelectrochemical systems.

CO₂ can be used as a substrate to generate methane (CH₄) by using enriched methanogens or can be converted to metabolites with CH₄. Recently, there has been increasing interest in co-utilization of one-carbon compounds such as CH₄ or CO₂ as substrates, not only because of their abundance, but also because both are produced from conventional anaerobic digestion of waste materials. Moving forward, opportunities to perform comparative analyses would allow studying a broad range of technologies converting CO₂ and CH₄ to fuels and chemicals to understand their potential economic and environmental benefits on previous or ongoing biomass conversion pathways funded by BETO. Specifically, process feasibility and TEA modeling for waste gaseous carbon utilization within integrated biorefinery systems such as this would allow for understanding technical performance

levels that would be required to offset the added costs for such operations in order to realize net economic benefits to the biorefinery. Gaining better understanding of new reaction mechanisms and opportunities to optimize carbon flux/energy efficiency may allow for highlighting paths to improved economics and relaxing targets for other challenging parameters elsewhere in the integrated process.

Methane to Products

Similar to the above concept, microbial conversion of biogas using natural CH₄-consuming bacteria (methanotrophs) offers broad and highly selective valorization potential. Methanotrophic bacteria are characterized by their ability to utilize a variety of different C1 substrates, including biogas generated from wastewater treatment facilities, as sole carbon and energy sources. Previous research using methanotrophic bacteria has demonstrated production of lactic acid, muconic acid, succinic acid, acetic acid, formic acid, and lipids [159-161]. NREL researchers have explored numerous methane to chemical pathways through process and market analyses and recommended several chemical intermediates for future R&D, including microbial biomass, sucrose, butanediol, succinic acid, and additional hydrocarbon fuel intermediates (NREL unpublished results). A series of process configurations are planned to be investigated for insertion of biogas fermentation into current process designs, with gas fermentation products serving as inputs at different locations, including (a) biomass pretreatment, (b) biological conversion, (c) product upgrading, or (d) coproduct production to increase overall biorefinery carbon efficiency.

Although the present design configuration has eliminated the anaerobic digestion unit from the WWT system (and thus the primary source of biogas), this is primarily a reflection of the aggressive assertions made around the lignin/residuals upgrading train (Area 700) and the high targeted conversions of all components that were previously relegated to WWT. In the event such high conversions could not be achieved or a different configuration strategy was pursued (as outlined below), the COD loading to the WWT system would increase again, which could require re-introducing the anaerobic digestion (AD) unit. Thus, as a “risk mitigation strategy” it will be useful moving forward to evaluate AD biogas utilization opportunities for increased carbon retention and improved economics. One such option is sucrose production from biogas, utilizing bubble columns to capture and convert a portion of the biogas methane. The sucrose could subsequently be converted to fuel precursors at high utilization efficiencies through either the BDO or acid pathways or could alternatively be used in the lignin upgrading train to produce additional muconic acid coproduct. Alternatively, a more economical option may be to produce either the fuel or coproduct molecules directly in the biogas upgrading bioreactor without the sucrose intermediate, if sufficiently high yields and productivities could be achieved. Another option may also be directly selling the produced sucrose as a coproduct (although this would be relatively low-value being tied to sucrose market prices) or producing single-cell protein for animal feed markets.

Alternative Uses for Lignin/Carbohydrates

A key driver for meeting the out-year \$2.50/GGE cost goal is maximizing the utilization of all biomass constituents in a highly efficient and integrated conversion strategy. Given the importance of maximizing the value of biomass and valorizing all components, particularly lignin, further improvements to conversion yield and efficiency may be realized by utilizing alternative strategies for biomass deconstruction with one out-year option focused on a “lignin first” deconstruction method. While this concept is in an early stage of development, the ultimate objective of such an option is to maximize the removal and conversion of lignin while minimizing losses of carbohydrates. Removing

the recalcitrant portion of the biomass, such as lignin, has been shown to reduce pretreatment severity and reduce enzyme loading for sugar production. The deconstruction strategy chosen, however, must be tailored for downstream conversion. Chemical catalytic processes that integrate deconstruction of residual solids with catalytic upgrading, i.e. the RCF concepts discussed above, are targeting high-value chemicals and fuels from lignin [162-164]. Recent efforts have focused on improving both carbon selectivity and atom efficient conversion for these upgrading options, as well as driving down catalyst costs.

Alternatively, more traditional thermochemical routes such as pyrolysis also offer an additional opportunity to upgrade residual lignin to fuel blendstocks. These strategies for lignin conversion to fuels could also open up the opportunity to instead utilize sugars for the production of high-value chemical coproducts and further integrate with pathways being pursued under the DOE BETO-supported Agile BioFoundry project, which aims to advance early-stage metabolic science to accelerate the rate of strain improvements and to develop robust, scalable organisms for fuel and product manufacturing [165]. By focusing on a diverse spectrum of product options from both sugars and lignin across a range of upgrading strategies, these efforts have aimed to reduce the risk of saturating chemicals markets and depressing chemical prices while boosting the value of traditionally underutilized fractions of the biomass. Given the projected growth of the bio-industry and the number of biorefineries needed to meet out-year fuel production needs, a range of coproduct strategies will be required to help enable low-cost biofuels.

Finally, a more simplistic route to reduce MFSPs while maintaining the overall structure of the process configurations would be to divert a fraction of the sugar fermentation intermediates away to coproducts. To minimize costs and avoid introducing further process complexity through a third processing train to a completely different product, the most practical approach here would be to isolate products already being produced or which could easily be produced from the existing upgrading steps as value-added coproducts. In the case of BDO, logical choices could be 1,3-butadiene or MEK, both produced through dehydration reactions from 2,3-BDO (there is not a large market for the 2,3-BDO component itself, although there is a considerable market for 1,4-BDO). In the case of the acids pathway, isolating ketone intermediates (i.e., 4-heptanone) may present opportunities for sale into solvent markets or related products.

6 Concluding Remarks

6.1 Summary

This report establishes a plausible case for achieving an ultimate cost goal below \$2.50/GGE of upgraded renewable hydrocarbon fuels by 2030 via biological production, based on two conceptual integrated processing pathways to hydrocarbon fuels coupled with bio-derived coproducts. Namely, the models discussed here assume continued improvements are made in the biomass deconstruction areas, including more novel approaches to alkaline extraction and mechanical refining pretreatment, as well as (in one case) continuous enzymatic hydrolysis, beyond performance demonstrated in prior state of technology benchmarking efforts. This includes demonstrating high solubilization of lignin, extractives, acetate, ash, and other non-fermentable components while minimizing losses of fermentable components and maximizing concentration of DMR black liquor through the use of a counter-current alkaline extraction operation. For the case of continuous enzymatic hydrolysis, this also includes demonstrating nearly 100% conversions of carbohydrates to monomeric sugars at a combined enzyme loading of 10 mg/g cellulose. These front-end unit operations leverage NREL expertise and prior work in these areas and will remain important areas of future research for continued improvement.

In addition to biomass deconstruction to sugars, the design also sets targets for sugar upgrading to fuels and importantly, lignin and other residual component upgrading to coproducts. On the former, two pathways to bioconversion intermediates are considered—carboxylic acids and 2,3-BDO, both under high sugar conversion efficiencies (95% glucose, 85%–90% xylose, and 85% arabinose to products) and intermediate product yields (>88% of theoretical). These intermediates are subsequently routed through catalytic upgrading reactions to expand chain lengths to fuel-range components as well as deoxygenate/hydrogenate the catalytic intermediates to finished hydrocarbon products, with high targeted yield and selectivity to desired fuel products. In light of the high demands and resultant costs for caustic and acid inputs throughout the process (contributing roughly \$1.30/GGE to overall MFSPs), it will be critical to either recover and recycle the majority of these chemicals through advanced separation technologies or to offset a fraction of those costs through the sale of resultant sodium sulfate salt isolated downstream, with this model reflecting the latter approach (at an average coproduct savings of roughly \$0.54/GGE, offsetting approximately 40% of the raw chemical costs in either pathway).

The majority of all biological and catalytic upgrading steps for both fuel train scenarios have largely been demonstrated at performance levels that support meeting final targets by 2030 and in many cases sooner, reflective of paths to first achieve \$3/GGE interim goals by 2022 prior to final goals below \$2.50/GGE by 2030. However, the targets set forward for the lignin-to-coproduct train represent newer research and may be reflective of a longer timescale closer to the final 2030 out-years, particularly with respect to lignin deconstruction to convertible monomers, targeted at 53% of the original biomass lignin (inclusive of both deconstruction across DMR pretreatment as well as subsequently across BCD in the lignin train). After that point, lignin train bioconversion and product recovery/upgrading are generally more straightforward based on performance observed to date, with targets set at 1 g/L-hr muconic acid productivity, 0.315 g/g muconic acid yield from lignin monomers, 0.93 g/g muconic acid yield from other residual components (extractives and carbohydrates), and 95% net recovery and conversion of muconic to adipic acid (inclusive of muconic and adipic acid purification as well as muconic acid hydrogenation).

The end result of the techno-economic analysis was a predicted MFSP of \$2.47/GGE for the BDO pathway and \$2.49/GGE for the acids pathway (2016\$) at a final upgraded fuel product yield of 43.2 and 44.8 GGE/dry ton of biomass for the two respective pathways. This reflects a \$1.65/GGE and \$1.59/GGE contribution from feedstock at \$71.26/dry ton, and a \$3.83/GGE and \$3.87/GGE contribution from the fuel train conversion process for the BDO and acids pathways, respectively. Critical to either pathway's ability to ultimately meet MFSPs below \$2.50/GGE is the inclusion of coproducts derived from lignin (and other residual components); in this work, adipic acid is reflected as a representative example coproduct with a targeted yield of 266 and 259 lb/dry ton, which translates to substantial coproduct offsets to the MFSP at *negative* \$3.00/GGE and \$2.97/GGE for the BDO and acids pathways, respectively. At those yields, the current global market for adipic acid (2.8 MM tonne/year) would be met with approximately 33 biorefineries of this size. However, we stress that adipic acid is intended to represent *one example* of many other potential products from lignin (or sugars), and in reality different biorefineries would be expected to produce different products as prevailing market conditions dictate, just as petrochemical facilities do not all produce the same products. In the more near term, in order to achieve interim MFSP goals of \$3/GGE by 2022, the majority of the fuel train targets are anticipated to likely still be achievable within that timeframe, which would relax the lignin coproduct assumptions to only require 235 and 229 lb/dry ton net adipic acid yields for the BDO and acids pathways, respectively (after adjusting feedstock costs to interim 2022 goals of \$79.07/dry ton). This translates primarily to reduced lignin deconstruction to monomers at roughly 43%, if simplistically focused on adjusting the single most challenging metric in isolation.

In addition to providing an economic analysis, the present report also considers key sustainability metric indicators that may be important factors in an overall LCA of the system. For the BDO pathway, these metrics were estimated at 25% carbon yield from biomass to fuels, 10.5 KWh/GGE net power import, 15.4 MJ/GGE natural gas consumption, and 8.9 gal/GGE net water demands for the biorefinery. For the acids pathway, these were estimated at 26% carbon yield, 10.7 KWh/GGE power import, 9.6 MJ/GGE natural gas consumption, and 13.5 gal/GGE net water demand. The coproduction of bio-derived adipic acid may provide substantial credits to overall biorefinery greenhouse gas emission profiles when compared to more energy-intensive fossil-derived synthesis for this product (dependent on LCA coproduct handling methods), but this is outside the scope of the present analysis.

The modeled selling prices are strictly representative of *nth*-plant assumptions regarding biorefinery design, operation, and financing, and are not intended to reflect first-of-a-kind or early-entry commercial facilities. While the fuel yields presented here are lower and the costs to produce those fuels are higher than what may be possible for cellulosic ethanol, the technology pathways described in this report are more representative of a true "biorefinery" that converts biomass to fungible hydrocarbon fuel products (which may be directly utilized by the existing fuel infrastructure), as well as advantaged bioproducts with relatively straightforward synthesis routes that leverage the compositional characteristics of the biomass feedstock. Within the context of such biorefinery concepts, additional alternative process integration strategies are also possible, including conversion of waste gaseous carbon for increased biorefinery carbon yields, or a number of different options for alternate processing approaches to convert lignin and/or carbohydrates to fuels or coproducts. These were not considered through rigorous TEA in the present scope but may be evaluated moving forward as additional risk mitigation strategies in meeting the \$2.50/GGE targets in the future. Given the relatively high capital expenses in this design to produce both hydrocarbon fuels and coproducts as required to achieve the \$2.50/GGE goal (roughly \$700MM or more TCI for both pathways), in the near-term it may be expected for early commercial pioneer facilities to focus on products alone to

reduce complexity and cost and improve overall process economics, in transitioning to products and fuels under n^{th} -plant scenarios.

It is worthwhile to reiterate that cellulosic ethanol production via fermentative pathways is supported by decades of research and process understanding, both at NREL and elsewhere, thus carrying a level of certainty and credibility when making target projections for biochemical ethanol TEA modeling, as in the case of the 2011 and even 2002 ethanol design reports. In contrast, biological hydrocarbon production is a much newer and more novel approach to biological conversion of sugars, with doors that have only recently been opened to a number of product pathways given recent advances in metabolic engineering, which continues to be a rapidly evolving field in this context. This point is even more relevant for lignin upgrading to coproducts, which is a challenge that has been studied for many years but has only recently demonstrated more substantial progress. Thus, the absolute cost values established here, as well as the timeframe required to achieve these outcomes, inherently carries a somewhat higher degree of uncertainty given the nascent stage of research as presented in the public domain.

6.2 Future Work

Moving forward, to ultimately achieve cost goals as well as reduce uncertainty in key areas for the modeled processes evaluated here, a number of important bottlenecks, uncertainties, and areas for further development are summarized below. A number of these points are similar to those raised in NREL's 2013 biological design case and remain equally pertinent here:

- **Investigate synergistic opportunities for biomass deconstruction/sugar production and process integration:** Tailoring the hydrolysate stream to the microorganism tolerance and bioreactor operation will be essential to improving yield and lowering production cost, and there continue to be further opportunities for synergistic improvement in combining unit operations or otherwise simplifying the fully integrated process. Moving to continuous enzymatic hydrolysis is one such example being better tailored to the acids pathway, which requires separating solids prior to bioconversion (otherwise incurring high costs for vacuum belt filtration with a flocculant), versus the BDO pathway which may process whole slurry hydrolysate through bioconversion and thus is better suited for standard batch hydrolysis. Additionally, more room exists for optimization and improved understanding of the proposed counter-current alkaline extraction unit currently envisioned in the DMR step.
- **Improve understanding of advanced bioreactor designs:** Both fuel train pathways have the potential to require more novel bioreactor designs and operating strategies, i.e., pertractive fermentation for the acids pathway and the potential for microaerophilic fermentation for the BDO pathway (in the event the organism cannot be engineered to eliminate oxygen redox balancing needs). Current design and cost estimates for such equipment are not as well established as more standard bioreactors for fully anaerobic or fully aerobic systems that NREL has considered in the past, and may benefit from further refinements moving forward.
- **Maximize sugar (and/or carbon) utilization and microbe metabolic performance:** Further work remains on strain engineering opportunities for the *Z. mobilis* BDO organism with respect to improving xylose/arabinose uptake, minimizing side-product formation, and eliminating oxygen demands to be replaced with alternative options for cell redox balancing (such as coproduction of hydrogen or succinic acid). Similarly, the *Clostridium* acids organism

also may have further room for improvement on the former two metrics, and more importantly on demonstrating cost-effective fermentation approaches avoiding costly pH control (e.g., pertractive acids recovery, low-pH tolerant organisms, or pH control with subsequent salt recovery strategies). Better understanding is needed as to optimal sugar concentrations in both fermentation pathways, and potential effects of hydrolysate inhibitors. Likewise, more work remains with the *P. putida* organism for lignin monomer (and other available components) fermentation with respect to integrating the multiple metabolic strategies into one single strain and reducing the impact of native regulatory responses preventing desired co-consumption behavior. Additionally, further metabolic modeling and fermentation optimization assessing the tradeoffs in yield versus productivity provides a process-oriented opportunity for improvement (e.g., fed-batch, reactor design, nutrient demands, substrate concentrations, etc.).

- **Improve catalyst performance for intermediate upgrading:** The present pathway models include a number of catalysis steps for upgrading both the fuel and coproduct intermediates. Current research is ongoing, but generally still in a relatively early state of development, around the majority of the catalytic upgrading steps considered here with respect to reactor operating conditions, space velocities, yields, selectivities, and catalyst material costs (efforts that are primarily coordinated under the ChemCatBio Consortium). As further details on such performance metrics and opportunities for future optimization emerge, the models will be refined accordingly, and improvements may be reflected in future state of technology benchmarks. Furthermore, the potential for refinery integration has not been extensively investigated for these biochemically derived intermediate components, and there may be opportunities for further cost reduction in pursuing such integration strategies, i.e., for final hydrotreating steps of the fuel precursor components to be handled centrally in a refinery rather than at a much smaller scale for these modeled facilities.
- **Improve lignin deconstruction and upgrading metrics:** The primary challenge of the lignin conversion targets set forth here will be effective lignin deconstruction to convertible monomers, thus this metric in particular deserves further attention and research on further optimization possibilities. Additionally, the present model is challenged by the granularity in characterization of the lignin monomer/oligomer properties and composition. While generally, lignin will proceed through the current valorization scheme regardless of specific chemical monomer structure (e.g., vanillin, ferulic acid, p-coumarate, etc.), both the deconstruction to monomers and the subsequent biological upgrading to muconic acid will display variations based on the specific makeup of soluble lignin. For example, during the aerobic upgrading, variations in oxidation state and the number of oxygen atoms on the monomer will play a role in the amount of oxygen demands, which can be a major cost driver.
- **Evaluate alternative integration strategies:** Alternate integration strategies may also provide new routes to the MFSP targets presented here, which were not evaluated in the present work but may be considered moving forward. These may include alternative approaches for lignin fractionation and/or thermochemical conversion to fuels or products, thus unlocking other options for sugars to instead be routed to products; or alternatively, pursuing utilization of waste gaseous streams for conversion to additional fuel/product opportunities.

References

NREL milestone reports cited below cannot be accessed outside of NREL and DOE. Readers may contact the authors of the specific reference to determine if this information has been made public since publication of this design report.

1. Wooley, R.J., M. Ruth, J. Sheehan, K. Ibsen, and H. Majdeski, A. Galvez. 1999. *Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis Current and Futuristic Scenarios*. NREL/TP-580-26157. Golden, CO: National Renewable Energy Laboratory.
2. Humbird, D., R. Davis, L. Tao, C. Kinchin, D. Hsu, A. Aden, P. Schoen, J. Lukas, B. Olthof, M. Worley, D. Sexton, and D. Dudgeon. 2011. *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol: Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover*. NREL/TP-5100-47764. Golden, CO: National Renewable Energy Laboratory.
3. Aden, A., M. Ruth, K. Ibsen, J. Jechura, K. Neeves, J. Sheehan, B. Wallace, L. Montague, A. Slayton, and J. Lukas. 2002. *Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic Hydrolysis for Corn Stover*. NREL/TP-510-32438. Golden, CO: National Renewable Energy Laboratory.
4. Schell, D. 2013. "Biochemical Processing Integration." Presented at the DOE Bioenergy Technologies Office Project Peer Review, Alexandria, Virginia, May 20–24, 2013.
5. Davis, R. 2013. "Biochemical Platform Analysis." Presented at the DOE Bioenergy Technologies Office Project Peer Review, Alexandria, Virginia, May 20–24, 2013.
6. Tao, L., et al. 2012. "FY 2012 Biochemical Platform State of Technology Report." NREL milestone report.
7. Tao, L., D. Schell, R. Davis, E. Tan, R. Elander, and A. Bratis. 2014. *NREL 2012 Achievement of Ethanol Cost Targets: Biochemical Ethanol Fermentation via Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover*. NREL/TP-5100-61563. Golden, CO: National Renewable Energy Laboratory.
8. U.S. Department of Energy. 2013. *Bioenergy Technologies Office Multi-Year Program Plan*. Washington, DC: U.S. Department of Energy.
9. Davis, R., L. Tao, C. Scarlata, E.C.D. Tan, J. Ross, J. Lukas, and D. Sexton. 2015. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons: Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Catalytic Conversion of Sugars to Hydrocarbons*. NREL/TP-5100-62498. Golden, CO: National Renewable Energy Laboratory.
10. Davis, R., L. Tao, E.C.D. Tan, M J. Bidy, G.T. Beckham, C. Scarlata, and J. Jacobson, et al. 2013. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons-Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Biological*

Conversion of Sugars to Hydrocarbons. NREL/TP-5100-60223. Golden, CO: National Renewable Energy Laboratory.

11. Bidy, M.J., C. Scarlata, and C. Kinchin. 2016. *Chemicals from Biomass: A Market Assessment of Bioproducts with Near-Term Potential*. NREL/TP-5100-65509. Golden, CO: National Renewable Energy Laboratory.
12. Davis, R. 2017. "Biochemical Platform Analysis." Presented at the DOE Bioenergy Technologies Office Project Peer Review, Denver, Colorado, March 7, 2017.
13. Humbird, D., R. Davis, and J. McMillan. 2017. "Aeration costs in stirred-tank and bubble column bioreactors." *Biochemical Engineering Journal* 127: 161–166. <https://doi.org/10.1016/j.bej.2017.08.006>.
14. Yang, Shihui, Ali Mohagheghi, Mary Ann Franden, Yat-Chen Chou, Xiaowen Chen, Nancy Dowe, Michael E. Himmel, and Min Zhang. 2016. "Metabolic engineering of *Zymomonas mobilis* for 2, 3-butanediol production from lignocellulosic biomass sugars." *Biotechnology for Biofuels* 9, no. 1: 189. <https://dx.doi.org/10.1186%2Fs13068-016-0606-y>.
15. AspenPlus (Release 7.2). 2007. Cambridge, MA: Aspen Technology Inc.
16. Christensen, Peter, and Larry R. Dysert. 2016. *Cost Estimate Classification System – As Applied in Engineering, Procurement, and Construction for the Process Industries, 18R-97*. Morgantown, WV: AACE International.
17. Cran, J. 1981. "Improved factored method gives better preliminary cost estimates." *Chemical Engineer* 88, no. 7: 65–79.
18. Wooley, R.J., V. Putsche, and K. Ibsen. 1999. *Development of an ASPEN PLUS Physical Property Database for Biofuels Components*. NREL Technical Memo, Document #4141. Golden, CO: National Renewable Energy Laboratory: Golden, CO.
19. Wooley, R.J. and V. Putsche. 1996. *Development of an ASPEN PLUS Physical Property Database for Biofuels Components*. NREL/TP-425-20685. Golden, CO: National Renewable Energy Laboratory: Golden, CO.
20. Hess, J.R. 2010. "Uniform Format Design and Depot Preprocessing." Presented at the Pacific NorthWest Economic Region's 2010 Annual Summit, Calgary, Alberta, July 16-20, 2010.
21. Chen, Shou-Feng, Richard A. Mowery, Christopher J. Scarlata, and C. Kevin Chambliss. 2007. "Compositional analysis of water-soluble materials in corn stover." *Journal of Agricultural and Food Chemistry* 55, no. 15: 5912–5918. <https://dx.doi.org/10.1021/jf0700327>
22. U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Fuel Cell Technologies Office. 2012. "Lower and higher heating values of fuels." <https://h2tools.org/hyarc/calculator-tools/lower-and-higher-heating-values-fuels>.

23. U.S. Department of Energy. 2016. *2016 Billion-Ton Report: Advancing Domestic Resources for a Thriving Bioeconomy*. Langholtz, M., B. Stokes, and L. Eaton, leads. ORNL/TM-2016/160. Oak Ridge, TN: Oak Ridge National Laboratory.
24. Bonner, Ian J., Kara G. Cafferty, David J. Muth, Jr., Mark D. Tomer, David E. James, Sarah A. Porter, and Douglas L. Karlen. 2014. "Opportunities for energy crop production based on subfield scale distribution of profitability." *Energies* 7, no. 10: 6509–6526. <https://dx.doi.org/10.3390/en7106509>.
25. Ssegane, Herbert, M., Cristina Negri, John Quinn, and Meltem Urgan-Demirtas. 2015. "Multifunctional landscapes: Site characterization and field-scale design to incorporate biomass production into an agricultural system." *Biomass and Bioenergy* 80: 179–190. <https://doi.org/10.1016/j.biombioe.2015.04.012>.
26. Stoof, Cathelijne R., Brian K. Richards, Peter B. Woodbury, Eric S. Fabio, Alice R. Brumbach, Jerry Cherney, and Srabani Das, et al. 2015. "Untapped potential: opportunities and challenges for sustainable bioenergy production from marginal lands in the Northeast USA." *BioEnergy Research* 8, no. 2: 482–501. <https://doi.org/10.1007/s12155-014-9515-8>.
27. Werling, Ben P., Timothy L. Dickson, Rufus Isaacs, Hannah Gaines, Claudio Gratton, Katherine L. Gross, and Heidi Liere, et al. 2014. "Perennial grasslands enhance biodiversity and multiple ecosystem services in bioenergy landscapes." *Proceedings of the National Academy of Sciences* 111, no. 4: 1652–1657. <https://doi.org/10.1073/pnas.1309492111>.
28. Dauber, J., C. Brown, A. L. Fernando, J. Finnan, E. Krasuska, J. Ponitka, and D. Styles, et al. 2012. "Bioenergy from 'surplus' land: environmental and socio-economic implications." *BioRisk – Biodiversity and Ecosystem Risk Assessment* 7: 5–50. <https://doi.org/10.3897/biorisk.7.3036>.
29. Valentine, John, John Clifton-Brown, Astley Hastings, Paul Robson, Gordon Allison, and Pete Smith. 2012. "Food vs. fuel: the use of land for lignocellulosic 'next generation' energy crops that minimize competition with primary food production." *GCB Bioenergy* 4, no. 1: 1–19. <https://doi.org/10.1111/j.1757-1707.2011.01111.x>.
30. Lacey, Jeffrey A., John E. Aston, Tyler L. Westover, Robert S. Cherry, and David N. Thompson. 2015. "Removal of introduced inorganic content from chipped forest residues via air classification." *Fuel* 160: p. 265–273. <https://doi.org/10.1016/j.fuel.2015.07.100>.
31. Thompson, Vicki S., Jeffrey A. Lacey, Damon Hartley, Michael A. Jindra, John E. Aston, and David N. Thompson. 2016. "Application of air classification and formulation to manage feedstock cost, quality and availability for bioenergy." *Fuel* 180: 497–505. <https://doi.org/10.1016/j.fuel.2016.04.040>.
32. Lacey, Jeffrey A., Rachel M. Emerson, David N. Thompson, and Tyler L. Westover. 2016. "Ash reduction strategies in corn stover facilitated by anatomical and size fractionation." *Biomass and Bioenergy* 90: 173–180. <https://doi.org/10.1016/j.biombioe.2016.04.006>.

33. Yancey, N., C.T. Wright, and T.L. Westover. 2013. "Optimizing hammer mill performance through screen selection and hammer design." *Biofuels* 4, no. 1: 85–94. <https://doi.org/10.4155/bfs.12.77>.
34. Aston, John E., David N. Thompson, and Tyler L. Westover. 2016. "Performance assessment of dilute-acid leaching to improve corn stover quality for thermochemical conversion." *Fuel* 186: 311–319. <https://doi.org/10.1016/j.fuel.2016.08.056>.
35. Tumuluru, J.S. 2014. "Effect of process variables on the density and durability of the pellets made from high moisture corn stover." *Biosystems Engineering* 119: 44–57. <https://doi.org/10.1016/j.biosystemseng.2013.11.012>.
36. Tumuluru, J.S. 2015. "High moisture corn stover pelleting in a flat die pellet mill fitted with a 6 mm die: physical properties and specific energy consumption." *Energy Science & Engineering* 3, no. 4: 327–341. <https://doi.org/10.1002/ese3.74>.
37. Tumuluru, J.S. 2016. "Specific energy consumption and quality of wood pellets produced using high-moisture lodgepole pine grind in a flat die pellet mill." *Chemical Engineering Research and Design* 110: 82–97. <https://doi.org/10.1016/j.cherd.2016.04.007>.
38. Tumuluru, J.S., C.C. Conner, and A.N. Hoover. 2016. "Method to produce durable pellets at lower energy consumption using high moisture corn stover and a corn starch binder in a flat die pellet mill." *Journal of Visualized Experiments* 112. <https://doi.org/10.3791/54092>.
39. Tumuluru, J.S. 2017. "Biomass Engineering, Size Reduction, Drying and Densification of High-Moisture Biomass." Presented at the DOE Bioenergy Technologies Office Project Peer Review, Denver, Colorado, March 7, 2017.
40. Tao, L., D. Schell, R. Davis, E. Tan, R. Elander, and A. Bratis. 2014. *NREL 2012 Achievement of Ethanol Cost Targets: Biochemical Ethanol Fermentation via Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover*. NREL/TP-5100-61563. Golden, CO: National Renewable Energy Laboratory.
41. Chen, Xiaowen, Erik Kuhn, Edward W. Jennings, Robert Nelson, Ling Tao, Min Zhang, and Melvin P. Tucker. 2016. "DMR (deacetylation and mechanical refining) processing of corn stover achieves high monomeric sugar concentrations (230 g L⁻¹) during enzymatic hydrolysis and high ethanol concentrations (> 10% v/v) during fermentation without hydrolysate purification or concentration." *Energy & Environmental Science* 9, no. 4: 1237–1245. <https://doi.org/10.1039/C5EE03718B>.
42. Chen, Xiaowen, Joseph Shekiri, Thomas Pschorn, Marc Sabourin, Melvin P. Tucker, and Ling Tao. 2015. "Techno-economic analysis of the deacetylation and disk refining process: characterizing the effect of refining energy and enzyme usage on minimum sugar selling price and minimum ethanol selling price." *Biotechnology for Biofuels* 8, no. 1: 173. <https://dx.doi.org/10.1186/s13068-015-0358-0>.

43. Chen, X., et al. 2014. "Produce 2 kg each of 3 different deacetylated/mechanically refined/enzyme digested lignin rich corn stover residues for a joint milestone with the Lignin Utilization task for analysis and depolymerization." NREL Milestone Report.
44. Chen, Xiaowen, Erik Kuhn, Nick Nagle, Rob Nelson, Ling Tao, Nathan Crawford, and Melvin Tucker. 2018. "Recycling of Dilute Deacetylation Black Liquor to Enable Efficient Recovery and Reuse of Spent Chemicals and Biomass Pretreatment Waste." *Frontiers in Energy Research* 6: 51. <https://dx.doi.org/10.3389/fenrg.2018.00051>
45. Perry, R.H., D.W. Green, and J.O. Maloney. 1997. *Perry's Chemical Engineers' Handbook, 7th Edition*. New York: McGraw-Hill.
46. Bowen, E., S.C. Kennedy, and K. Miranda. 2010. "Ethanol from Sugar Beets: A Process and Economic Analysis." For the Degree of Bachelor of Science, Worcester Polytechnic Institute.
47. Stickel, Jonathan J., Birendra Adhikari, David A. Sievers, and John Pellegrino. 2017. "Continuous enzymatic hydrolysis of lignocellulosic biomass in a membrane-reactor system." *Journal of Chemical Technology and Biotechnology* 93, no. 8: 2181–2190. <https://doi.org/10.1002/jctb.5559>.
48. Fagerson, I. S. 1969. "Thermal degradation of carbohydrates; a review." *Journal of Agricultural and Food Chemistry* 17, no. 4: 747–750. <https://doi.org/10.1021/jf60164a019>.
49. Meerman, H.J., A.S. Kelley, and M. Ward. 2004. "Advances in Protein Expression in Filamentous Fungi." In *Protein Expression Technologies: Current Status and Future Trends*, edited by F. Baneyx. Norfolk, UK: Horizon Bioscience.
50. Warzywoda, M., et al., U.S. Patent No. 4,762,788, 28 November 1984.
51. Emme, B., Personal communication with D. Humbird. 2009.
52. Atkinson, B. and F. Mavituna. 1991. *Biochemical Engineering and Biotechnology Handbook*. New York: Stockton Press.
53. Schell, D., C. Riley, P. Bergeron, and P. Walter. 1991. *Technical and Economic Analysis of an Enzymatic Hydrolysis Based Ethanol Plant*. SERI/TP-232-4295. Golden, CO: Solar Energy Research Institute.
54. Humbird, D., et al. 2015. "Aeration cost and performance in STR and BC." NREL milestone report.
55. McMillan, J., et al. 2014. "Assessment of large-scale aeration economics." NREL milestone report.
56. Crater, J., C. Galleher, and J. Lievens. 2017. *Consultancy on Large-Scale Submerged Aerobic Cultivation Process Design – Final Technical Report*. NREL/SR-5100-67963. Golden, CO: National Renewable Energy Laboratory.

57. Ledesma-Amaro, Rodrigo, Remi Dulermo, Xochitl Niehus, and Jean-Marc Nicauda. 2016. "Combining metabolic engineering and process optimization to improve production and secretion of fatty acids." *Metabolic Engineering* 38: 38–46. <https://doi.org/10.1016/j.ymben.2016.06.004>.
58. Shumaker, Andrew M., Bernardo M. da Costa, Kevin Holden, Louis G. Hom, Tarah S. Baron, and Noah Helman. 2018. "Enzyme variants with improved ester synthase properties." U.S. Patent No. 9879239B2.
59. Qiao, Kangjian, Thomas M. Wasylenko, Kang Zhou, Peng Xu, and Gregory Stephanopoulos. 2017. "Lipid production in *Yarrowia lipolytica* is maximized by engineering cytosolic redox metabolism." *Nature Biotechnology* 35, no.2: 173. <https://doi.org/10.1038/nbt.3763>.
60. Meadows, Adam L., Kristy M. Hawkins, Yoseph Tsegaye, and Annie E. Tsong. 2016. "Rewriting yeast central carbon metabolism for industrial isoprenoid production." *Nature* 537, no. 7622: 694. <http://dx.doi.org/10.1038/nature19769>.
61. Zhang, M., et al. 2015. "Down select best gene combination to demonstrate 2,3-BDO production at 10 g/L in *Zymomonas mobilis* from glucose and xylose." NREL Milestone Report.
62. Zhang, M., et al. 2016. "Demonstrate production of 2,3 butanediol at 20 g/L using engineered *Zymomonas mobilis* from glucose and xylose derived from DMR-EH biomass hydrolysate." NREL Milestone Report.
63. Zhang, M., Y.-C. Chou, and A. Mohagheghi. 2017. "Demonstrate production of 2,3-butanediol from glucose & xylose at 35 g/L using engineered *Zymomonas mobilis* using batch and/or fed-batch fermentations." NREL Milestone Report.
64. Davis, R., M. Bidy, and L. Tao. 2017. "Catalytic Pathway Alternatives: Conduct TEA modeling on at least two additional pathways for catalytic upgrading of hydrolysate intermediates, beyond the 'catalytic conversion of sugars' design case focused on APR." NREL Milestone Report.
65. Davis, R., et al. 2017. "Options to support \$2/GGE." NREL Milestone Report.
66. Davis, R., L. Tao, C. Scarlata, E.C.D. Tan, J. Ross, J. Lukas, and D. Sexton. 2015. *Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons Dilute-Acid and Enzymatic Deconstruction of Biomass to Sugars and Catalytic Conversion of Sugars to Hydrocarbons*. NREL/TP-5100-62498. Golden, CO: National Renewable Energy Laboratory.
67. Ji, X.-J., H. Huang, and P.-K. Ouyang. 2011. "Microbial 2,3-butanediol production: A state-of-the-art review." *Biotechnology Advances* 29, no. 3: 351–364. <https://doi.org/10.1016/j.biotechadv.2011.01.007>.
68. Xiu, Z.-L. and A.-P. Zeng. 2008. "Present state and perspective of downstream processing of biologically produced 1,3-propanediol and 2,3-butanediol." *Applied Microbiology and Biotechnology* 78, no. 6: 917–926. <https://doi.org/10.1007/s00253-008-1387-4>.
69. Davis, R., et al. 2016. "TEA Identification of Most Promising Options for 2022 Targets." NREL milestone report.

70. Narula, Chaitanya, Zhenglong Li, Erik Casbeer, Robert Geiger, Melanie Moses-Debusk, Martin Keller, Michelle Buchanan, and Brian Davison. 2015. "Heterobimetallic zeolite, InV-ZSM-5, enables efficient conversion of biomass derived ethanol to renewable hydrocarbons." *Scientific Reports* 5: 16039. <http://dx.doi.org/10.1038/srep16039>.
71. Li, Zhenglong, Oak Ridge National Laboratory, personal communication, 2018.
72. Zheng, Quanxing, Michael D. Wales, Michael G. Heidlage, Mary Rezac, Hongwang Wang, Stefan H. Bossmann, and Keith L. Hohn. 2015. "Conversion of 2, 3-butanediol to butenes over bifunctional catalysts in a single reactor." *Journal of Catalysis* 330: 222–237. <https://doi.org/10.1016/j.jcat.2015.07.004>.
73. Twigg, M.V. 1989. *Catalyst Handbook*, edited by M.V. Twigg. London: Wolfe.
74. Zhang, Xin, Jin Zhong, Jianwei Wang, Linhui Zhang, Junkui Gao, and Aisong Liub. 2009. "Catalytic performance and characterization of Ni-doped HZSM-5 catalysts for selective trimerization of n-butene." *Fuel Processing Technology* 90, no. 7–8: 863–870. <https://doi.org/10.1016/j.fuproc.2009.04.011>.
75. Golombok, M., and J. De Bruijn. 2000. "Density Variations in a Reactor During Liquid Full Dimerization." *Chemical Engineering Research and Design* 78, no. 1: 145–147. <https://doi.org/10.1205/026387600526988>.
76. Golombok, M., and J. de Bruijn. 2001. "Catalysts for producing high octane-blending value olefins for gasoline." *Applied Catalysis A: General* 208, no. 1–2: 47–53. [https://doi.org/10.1016/S0926-860X\(00\)00684-0](https://doi.org/10.1016/S0926-860X(00)00684-0).
77. Wright, M.E., B.G. Harvey, and R.L. Quintana. 2015. "Diesel and Jet Fuels Based on the Oligomerization of Butene." U.S. Patent No. 9,181,144.
78. Blommel, Paul, Brice Dally, Warren Lyman, and Randy Cortright. "Method and systems for making distillate fuels from biomass." International Patent Application No. WO2012109241.
79. Choi, Kieun, Byoung Seung Jeon, Byung-Chun Kim, Min-Kyu Oh, Youngsoon Um, and Byoung-In Sang. 2013. "In situ biphasic extractive fermentation for hexanoic acid production from sucrose by *Megasphaera elsdenii* NCIMB 702410." *Applied Biochemistry and Biotechnology* 171, no. 5: 1094–1107. <https://doi.org/10.1007/s12010-013-0310-3>.
80. Jiang, X.-l., S. Yong, and W.-y. Zhu. 2016. "Fermentation characteristics of *Megasphaera elsdenii* J6 derived from pig feces on different lactate isomers." *Journal of Integrative Agriculture* 15, no. 7: 1575–1583. [https://doi.org/10.1016/S2095-3119\(15\)61236-9](https://doi.org/10.1016/S2095-3119(15)61236-9).
81. Hashizume, Kenta, Takamitsu Tsukahara, Kouji Yamada, Hironari Koyama, and Kazunari Ushida. 2003. "*Megasphaera elsdenii* JCM1772T normalizes hyperlactate production in the large intestine of fructooligosaccharide-fed rats by stimulating butyrate production." *The Journal of Nutrition* 133, no. 10: 3187–3190. <https://doi.org/10.1093/jn/133.10.3187>.

82. Roddick, F.A. and M.L. Britz. 1997. "Production of hexanoic acid by free and immobilised cells of *Megasphaera elsdenii*: influence of in-situ product removal using ion exchange resin." *Journal of Chemical Technology & Biotechnology* 69, no. 3: 383–391. [https://doi.org/10.1002/\(SICI\)1097-4660\(199707\)69:3<383::AID-JCTB723>3.0.CO;2-H](https://doi.org/10.1002/(SICI)1097-4660(199707)69:3<383::AID-JCTB723>3.0.CO;2-H).
83. Nelson, Robert S, Darren J. Peterson, Eric M. Karp, Gregg T. Beckham, and Davinia Salvachúa. 2017. "Mixed carboxylic acid production by *Megasphaera elsdenii* from glucose and lignocellulosic hydrolysate." *Fermentation* 3, no. 1: 10. <https://doi.org/10.3390/fermentation3010010>.
84. Lee, Joungmin, Yu-Sin Jang, Mee-Jung Han, Jin Young Kim, and Sang Yup Lee. 2016. "Deciphering *Clostridium tyrobutyricum* metabolism based on the whole-genome sequence and proteome analyses." *MBio* 7, no. 3: e00743–16. <https://doi.org/10.1128/mBio.00743-16>.
85. Liu, X., Y. Zhu, and S.-T. Yang. 2006. "Butyric acid and hydrogen production by *Clostridium tyrobutyricum* ATCC 25755 and mutants." *Enzyme and Microbial Technology* 38 no. 3–4: 521–528. <https://doi.org/10.1016/j.enzmictec.2005.07.008>.
86. Zhu, Y., and S.-T. Yang. 2004. "Effect of pH on metabolic pathway shift in fermentation of xylose by *Clostridium tyrobutyricum*." *Journal of Biotechnology* 110, no. 2: 143–157. <https://doi.org/10.1016/j.jbiotec.2004.02.006>.
87. Russell, J. 1992. "Another explanation for the toxicity of fermentation acids at low pH: anion accumulation versus uncoupling." *Journal of Applied Microbiology* 73, no. 5: 363–370. <https://doi.org/10.1111/j.1365-2672.1992.tb04990.x>.
88. Zígová, Jana, Ernest Šturdík, Dušan Vandák, and Štefan Schlosser. 1999. "Butyric acid production by *Clostridium butyricum* with integrated extraction and pertraction." *Process Biochemistry* 34, no. 8: 835–843. [https://doi.org/10.1016/S0032-9592\(99\)00007-2](https://doi.org/10.1016/S0032-9592(99)00007-2).
89. Kawabata, N., J.-i. Yoshida, and Y. Tanigawa. 1981. "Removal and recovery of organic pollutants from aquatic environment. 4. Separation of carboxylic acids from aqueous solution using crosslinked poly (4-vinylpyridine)." *Industrial & Engineering Chemistry Product Research and Development* 20, no. 2: 386–390. <https://doi.org/10.1021/i300002a030>.
90. Kertes, A., and C.J. King. 1986. "Extraction chemistry of fermentation product carboxylic acids." *Biotechnology and Bioengineering* 28, no. 2: 269–282. <https://doi.org/10.1002/bit.260280217>.
91. Schlosser, Š., R. Kertész, and J. Martak. 2005. "Recovery and separation of organic acids by membrane-based solvent extraction and pertraction: An overview with a case study on recovery of MPCA." *Separation and Purification Technology* 41, no. 3: 237–266. <https://doi.org/10.1016/j.seppur.2004.07.019>.
92. Um, B.-H., B. Friedman, and G.P. van Walsum. 2011. "Conditioning hardwood-derived pre-pulping extracts for use in fermentation through removal and recovery of acetic acid using trioctylphosphine oxide (TOPO)." *Holzforchung* 65, no. 1: 51–58. <https://doi.org/10.1515/hf.2010.115>.

93. Wasewar, Kailas L., Archis A. Yawalkar, Jacob A. Moulijn, and Vishwas G. Pangarkar. 2004. "Fermentation of glucose to lactic acid coupled with reactive extraction: a review." *Industrial & Engineering Chemistry Research* 43, no. 19: 5969–5982. <https://doi.org/10.1021/ie049963n>.
94. Zhang, Chunhui, Hua Yang, Fangxiao Yang, and Yujiu Ma. 2009. "Current progress on butyric acid production by fermentation." *Current Microbiology* 59, no. 6: 656–663. <https://doi.org/10.1007/s00284-009-9491-y>.
95. Papoutsakis, E.T. 1984. "Equations and calculations for fermentations of butyric acid bacteria." *Biotechnology and Bioengineering* 26, no. 2: 174–187. <https://doi.org/10.1002/bit.260260210>.
96. Hano, Tadashi, Michiaki Matsumoto, Takaaki Ohtake, Kiyotaka Sasaki, Fumiaki Hori, and Yoshinobu Kawano. 1990. "Extraction equilibria of organic acids with tri-*n*-octylphosphineoxide." *Journal of Chemical Engineering of Japan*. 23, no. 6: 734–738. <https://doi.org/10.1252/jcej.23.734>.
97. Matsumoto, Michiaki, Shinji Uenoyama, Tadashi Hano, Makato Hirata, and Shigenobu Miura. 1996. "Extraction Kinetics of Organic Acids with Tri-*n*-octylphosphine Oxide." *Journal of Chemical Technology & Biotechnology* 67, no. 3: 260–264. [https://doi.org/10.1002/\(SICI\)1097-4660\(199611\)67:3<260::AID-JCTB559>3.0.CO;2-Y](https://doi.org/10.1002/(SICI)1097-4660(199611)67:3<260::AID-JCTB559>3.0.CO;2-Y).
98. Saboe, Patrick O., Lorenz P. Manker, William E. Michener, Darren J. Peterson, David G. Brandner, Stephen P. Deutch, Manish Kumar, Robin M. Cywar, Gregg T. Beckham, and Eric M. Karp. 2018. "In situ recovery of bio-based carboxylic acids." *Green Chemistry* 20, no. 8: 1791–1804. <https://doi.org/10.1039/C7GC03747C>.
99. Shylesh, Sankaranarayanapillai, Amit A. Gokhale, Keyang Sun, Adam M. Grippo, Deepak Jadhav, Alice Yeh, Christopher R. Hob, and Alexis T. Bell. 2017. "Integrated catalytic sequences for catalytic upgrading of bio-derived carboxylic acids to fuels, lubricants and chemical feedstocks." *Sustainable Energy & Fuels* 1, no. 8: 1805–1809. <https://doi.org/10.1039/C7SE00359E>.
100. Pham, Tu N., Tawan Sooknoi, Steven P. Crossley, and Daniel E. Resasco. 2013. "Ketonization of carboxylic acids: mechanisms, catalysts, and implications for biomass conversion." *ACS Catalysis* 3, no. 11: 2456–2473. <https://doi.org/10.1021/cs400501h>.
101. Moore, Cameron M., Rhodri W. Jenkins, Michael T. Janicke, William L. Kubic Jr., Evgueni Polikarpov, Troy A. Semelsberger, and Andrew D. Sutton. 2016. "Synthesis of Acetone-Derived C6, C9, and C12 Carbon Scaffolds for Chemical and Fuel Applications." *ChemSusChem* 9, no. 24: 3382–3386. <https://doi.org/10.1002/cssc.201600936>.
102. Sacia, Eric R., Madhesan Balakrishnan, Matthew H. Deaner, Konstantinos A. Goulas, F. Dean Toste, and Alexis T. Bell. 2015. "Highly Selective Condensation of Biomass-Derived Methyl Ketones as a Source of Aviation Fuel." *ChemSusChem* 8, no. 10: 1726–1736. <https://doi.org/10.1002/cssc.201500002>.
103. Aspen Technology. 2018. "Aspen Capital Cost Estimator." <https://www.aspentech.com/en/products/engineering/aspen-capital-cost-estimator>.

104. Datta, Saurav, Yupo J. Lin, Daniel J. Schell, C. S. Millard, Sabeen F. Ahmad, Michael P. Henry, P. Gillenwater, Anthony T. Fracaro, A. Moradia, Zofia P. Gwarnicki, and Seth W. Snyder. 2013. "Removal of Acidic Impurities from Corn Stover Hydrolysate Liquor by Resin Wafer Based Electrodeionization." *Industrial & Engineering Chemistry Research* 52, no. 38: 13777–13784. <https://doi.org/10.1021/ie4017754>.
105. Arora, M. B., J. A. Hestekin, S. W. Snyder, E. J. St. Martin, Y. J. Lin, M. I. Donnelly, and C. Sanville Millard. 2007. "The Separative Bioreactor: A Continuous Separation Process for the Simultaneous Production and Direct Capture of Organic Acids." *Sep Sci Technol* 42, no. 11: 2519–2538. <https://doi.org/10.1080/01496390701477238>.
106. Schutyser, W., T. Renders, S. Van den Bosch, S.-F. Koelewijn, G. T. Beckham, and B. F. Sels. 2018. "Chemicals from lignin: an interplay of lignocellulose fractionation, depolymerisation, and upgrading." *Chemical Society Reviews* 47, no. 3: 852–908. <https://doi.org/10.1039/C7CS00566K>.
107. Beckham, Gregg T., Christopher W. Johnson, Eric M. Karp, Davinia Salvachúa, and Derek R. Vardon. 2016. "Opportunities and challenges in biological lignin valorization." *Current Opinion in Biotechnology* 42: 40–53. <https://doi.org/10.1016/j.copbio.2016.02.030>.
108. Pavone, A. 2012. *Bio-Based Adipic Acid*. Santa Clara, CA: IHS Chemical.
109. Kojima, Yutaka, Hiroshi Fujisawa, Atsushi Nakazawa, Teruko Nakazawa, Fuminori Kanetsuna, Hiroshi Taniuchi, Mitsuhiro Nozaki, and Osamu Hayaishi. 1967 "Studies on Pyrocatechase I. Purification and Spectral Properties." *Journal of Biological Chemistry* 242, no. 14: 3270–3278.
110. Nakazawa, T. 2002. "Travels of a Pseudomonas from Japan around the world." *Environmental Microbiology* 4, no. 12: 782–786. <http://dx.doi.org/10.1046/j.1462-2920.2002.00310.x>.
111. Williams, P.A., and K. Murray. 1974. "Metabolism of benzoate and the methylbenzoates by *Pseudomonas putida* (arvilla) mt-2: evidence for the existence of a TOL plasmid." *Journal of Bacteriology* 120, no. 1: 416–423.
112. Nelson, K.E., C. Weinel, I.T. Paulsen, R.J. Dodson, H. Hilbert, V.A. Martins dos Santos, and D.E. Fouts, et al. 2002. "Complete genome sequence and comparative analysis of the metabolically versatile *Pseudomonas putida* KT2440." *Environmental Microbiology* 4, no. 12: 799–808. <https://doi.org/10.1046/j.1462-2920.2002.00366.x>.
113. Belda, Eugeni, Ruben G. A. van Heck, Maria José Lopez-Sanchez, Stéphane Cruveiller, Valérie Barbe, Claire Fraser, and Hans-Peter Klenk, et al. 2016. "The revisited genome of *Pseudomonas putida* KT2440 enlightens its value as a robust metabolic chassis." *Environmental Microbiology* 18 no. 10: 3403–3424. <https://doi.org/10.1111/1462-2920.13230>.
114. Linger, Jeffrey G., Derek R. Vardon, Michael T. Guarnieri, Eric M. Karp, Glendon B. Hunsinger, Mary Ann Franden, and Christopher W. Johnson, et al. 2014. "Lignin valorization through integrated biological funneling and chemical catalysis." *Proceedings of the National Academy of Sciences* 111, no. 33: 12013–12018. <https://doi.org/10.1073/pnas.1410657111>.

115. Thompson, B., M. Machas, and D.R. Nielsen. 2015. "Creating pathways towards aromatic building blocks and fine chemicals." *Current Opinion in Biotechnology* 36: 1–7. <https://doi.org/10.1016/j.copbio.2015.07.004>.
116. Burgard, A.P., P. Pharkya, and R.E. Osterhout. 2012. "Microorganisms for the production of adipic acid and other compounds." U.S. Patent No. 7799545B2.
117. Frost, J.W., and K.M. Draths. 1996. "Synthesis of adipic acid from biomass-derived carbon sources." U.S. Patent No. 5487987A.
118. Frost, J.W., and K.M. Draths. 1997. "Bacterial cell transformants for production of cis, cis-muconic acid and catechol." U.S. Patent No. 5616496A.
119. Niu, W., K. Draths, and J. Frost. 2002. "Benzene-Free Synthesis of Adipic Acid." *Biotechnology Progress* 18, no. 2: 201–211. <https://doi.org/10.1021/bp010179x>.
120. Yu, J.L., X.X. Xia, J.J. Zhong, and Z.G. Qian. 2014. "Direct biosynthesis of adipic acid from a synthetic pathway in recombinant *Escherichia coli*." *Biotechnology and Bioengineering* 111, no. 12: 2580–2586. <https://doi.org/10.1002/bit.25293>.
121. Johnson, Christopher W., Davinia Salvachúa, Payal Khanna, Holly Smith, Darren J. Peterson, and Gregg T. Beckham. 2016. "Enhancing muconic acid production from glucose and lignin-derived aromatic compounds via increased protocatechuate decarboxylase activity." *Metabolic Engineering Communications* 3: 111–119. <https://doi.org/10.1016/j.meteno.2016.04.002>.
122. Vardon, Derek R., Nicholas A. Rorrer, Davinia Salvachúa, Amy E. Settle, Christopher W. Johnson, Martin J. Menart, and Nicholas S. Cleveland, et al. 2016. "*cis, cis*-Muconic acid: separation and catalysis to bio-adipic acid for nylon-6, 6 polymerization." *Green Chemistry* 18, no. 11: 3397–3413. <https://doi.org/10.1039/C5GC02844B>.
123. Vardon, Derek R., Mary Ann Franden, Christopher W. Johnson, Eric M. Karp, Michael T. Guarnieri, Jeffrey G. Linger, Michael J. Salm, Timothy J. Strathmann, and Gregg T. Beckham. 2015. "Adipic acid production from lignin." *Energy & Environmental Science* 8, no. 2: 617–628. <https://doi.org/10.1039/C4EE03230F>.
124. Löwe, Hannes, Lukas Schmauder, Karina Hobmeier, Andreas Kremling, and Katharina Pflüger-Grau. 2017. "Metabolic engineering to expand the substrate spectrum of *Pseudomonas putida* toward sucrose." *MicrobiologyOpen* 6, no. 4. <https://doi.org/10.1002/mbo3.473>.
125. Orth, J.D., I. Thiele, and B.Ø. Palsson. 2010. "What is flux balance analysis?" *Nature Biotechnology* 28, no. 3: 245–248. <https://doi.org/10.1038/nbt.1614>.
126. Puchałka, J., et al. 2008. "Genome-scale reconstruction and analysis of the *Pseudomonas putida* KT2440 metabolic network facilitates applications in biotechnology." *PLoS computational biology* 4, no. 10: p. e1000210. <https://doi.org/10.1371/journal.pcbi.1000210>.
127. Jayakody, Lahiru N., Christopher W. Johnson, Jason M. Whitham, Richard J. Giannone, Brenna A. Black, Nicholas S. Cleveland, and Dawn M. Klingeman, et al. 2018. "Thermochemical

- wastewater valorization *via* enhanced microbial toxicity tolerance." *Energy & Environmental Science* 11, no. 6: 1625–1638. <https://doi.org/10.1039/C8EE00460A>.
128. Shiloach, J., and R. Fass. 2005. "Growing *E. coli* to high cell density—a historical perspective on method development." *Biotechnology Advances* 23, no. 5: 345–357. <https://doi.org/10.1016/j.biotechadv.2005.04.004>.
129. Van't Riet, K., and J. Tramper. 1991. *Basic Bioreactor Design*. Boca Raton, FL: CRC Press.
130. Gaivoronskii, A., and V. Granzhan. 2005. "Solubility of adipic acid in organic solvents and water." *Russian Journal of Applied Chemistry* 78, no. 3: [https://doi.org/404–408](https://doi.org/404-408). 10.1007/s11167-005-0305-0.
131. Scelfo, S., R. Pirone, and N. Russo. 2016. "Thermodynamics of cis, cis-muconic acid solubility in various polar solvents at low temperature range." *Journal of Molecular Liquids* 222: 823–827. <https://doi.org/10.1016/j.molliq.2016.07.129>.
132. Li, Qiang, Dan Wang, Yong Wu, Wangliang Li, Yunjian Zhang, Jianmin, Xing, and Zhiguo Su. 2010. "One step recovery of succinic acid from fermentation broths by crystallization." *Separation and Purification Technology* 72, no. 3: 294–300. <https://doi.org/10.1016/j.seppur.2010.02.021>.
133. Urbanus, J., C.P.M. Roelands, D. Verdoes, J.H. ter Horst. 2012. "Intensified crystallization in complex media: Heuristics for crystallization of platform chemicals." *Chemical Engineering Science* 77: 18–25. <https://doi.org/10.1016/j.ces.2012.02.019>.
134. Gary, J.H., G.E. Handwerk, and M.J. Kaiser. 2007. *Petroleum Refining: Technology and Economics*. Boca Raton, FL: CRC Press.
135. Nielsen, R.H. 2007. *Process Economics Program Report 214A: Heavy Oil Hydrotreating*. Menlo Park, CA: SRI Consulting.
136. Kaiser, M.J., and J.H. Gary. 2007. "Study updates refinery investment cost curves." *Oil & Gas Journal*, April 23, 2007. <https://www.ogj.com/articles/print/volume-105/issue-16/processing/study-updates-refinery-investment-cost-curves.html>.
137. Refining Process Services Inc. 2008. "Hydrotreating & Hydrocracking Process Technology Seminar." Presented in Houston, Texas, in 2008.
138. Palmer, E., S. Polcar, and A. Wong. 2009. "Clean Diesel Hydrotreating." *Petroleum Technology Quarterly* January 2009.
139. Guthrie, K.M. 1974. *Process Plant Estimating, Evaluation, and Control*. Carlsbad, CA: Craftsman Book Company of America.
140. Seider, W.D., J. Seader, and D.R. Lewin. 2004. *Product and Process Design Principles*. New York: Wiley.

141. Bray, R.G. 2007. *Process Economics Program Report 251A: Advances in Biodeisel and Renewable Diesel Production*. London: IHS Consulting.
142. Cesar, M. 2006. *Process Economics Program: Advances in Paraxylene Technology*. London: IHS Consulting.
143. Salvachúa, Davinia, Eric M. Karp, Claire T. Nimlos, Derek R. Vardon, and Gregg T. Beckham. 2015. "Towards lignin consolidated bioprocessing: simultaneous lignin depolymerization and product generation by bacteria." *Green Chemistry* 17, no. 11: 4951–4967. <https://doi.org/10.1039/C5GC01165E>
144. Rinaldi, Robert, Robin Jastrzebski, Matthew T. Clough, John Ralph, Marco Kennema, Pieter C. A. Bruijninx, and Bert M. Weckhuysen. 2016. "Paving the way for lignin valorisation: recent advances in bioengineering, biorefining and catalysis." *Angewandte Chemie International Edition* 55, no. 29: 8164–8215. <https://doi.org/10.1002/anie.201510351>.
145. Ragauskas, Arthur J., Gregg T. Beckham, Mary J. Bidy, Richard Chandra, Fang Chen, Mark F. Davis, and Brian H. Davison, et al. 2014. "Lignin valorization: improving lignin processing in the biorefinery." *Science* 344, no. 6185: 1246843. <https://doi.org/10.1126/science.1246843>
146. U.S. Department of Energy. 2016. *Bioenergy Technologies Office Multi-Year Program Plan*. Washington, DC: U.S. Department of Energy.
147. Chemical Engineering Magazine. 2011. "Chemical Engineering Magazine Plant Cost Index." http://folk.ntnu.no/magnehi/cepci_2011_py.pdf.
148. U.S. Bureau of Labor Statistics. 2009. "National Employment, Hours, and Earnings Catalog, Industry: Chemicals and Allied Products, 1980–2009." <http://data.bls.gov/cgi-bin/srgate>.
149. U.S. Department of Agriculture Economic Research Service. 2018. "Table 7—U.S. wholesale list price for glucose syrup, Midwest markets, monthly, quarterly, and by calendar and fiscal year." 2018. <https://www.ers.usda.gov/data-products/sugar-and-sweeteners-yearbook-tables.aspx>.
150. U.S. Energy Information Administration. 2015. "Electricity Data Browser-Average Retail Price of Electricity." <https://www.eia.gov/electricity/data/browser/>.
151. Dillich, S., T. Ramsden, and M. Melina. 2012. "Hydrogen Production Cost Using Low-Cost Natural Gas." DOE Hydrogen and Fuel Cells Program Record #12024. http://www.hydrogen.energy.gov/pdfs/12024_h2_production_cost_natural_gas.pdf
152. Steinwinder, Thomas, Everett Gill, and Matthew Gerhardt. 2012. *Process Design of Wastewater Treatment for the NREL Cellulosic Ethanol Model*. NREL/SR-5100-51838. Golden, CO: National Renewable Energy Laboratory.
153. Peters, Max, Klaus Timmerhaus, and Ronald West. 2003. *Plant Design and Economics for Chemical Engineers*. New York: McGraw-Hill.

154. SRI Consulting. 2008. "U.S. Producer Price Indexes – Chemicals and Allied Products/Industrial Inorganic Chemicals Index." In *Chemical Economics Handbook*. Menlo Park, CA: SRI Consulting.
155. Short, W., D.J. Packey, and T. Holt. 1995. *A Manual for the Economic Evaluation and Energy Efficiency and Renewable Energy Technologies*. NREL/TP-462-5173. Golden, CO: National Renewable Energy Laboratory.
156. Gary, J.H., and G.E. Handwerk. 1994. *Petroleum Refining: Technology and Economics, 3rd Edition*. New York: Marcel Dekker.
157. Bidy, Mary J., Ryan Davis, David Humbird, Ling Tao, Nancy Dowe, Michael T. Guarnieri, and Jeffrey G. Linger, et al. 2016. "The techno-economic basis for coproduct manufacturing to enable hydrocarbon fuel production from lignocellulosic biomass." *ACS Sustainable Chemistry & Engineering* 4, no. 6: 3196–3211. <https://doi.org/10.1021/acssuschemeng.6b00243>
158. Cai, Hao, Jeongwoo Han, Michael Wang, Ryan Davis, Mary Bidy, and Eric Tan. 2018. "Life-cycle analysis of integrated biorefineries with co-production of biofuels and bio-based chemicals: co-product handling methods and implications." *Biofuels, Bioproducts and Biorefining* 12, no. 5. <https://doi.org/10.1002/bbb.1893>.
159. Munasinghe, P.C., and S.K. Khanal. 2010. "Biomass-derived syngas fermentation into biofuels: Opportunities and challenges." *Bioresource Technology* 101, no. 13: 5013–5022. <https://doi.org/10.1016/j.biortech.2009.12.098>.
160. Fei, Qiang, Aaron W. Puri, Holly Smith, Nancy Dowe, and Philip T. Pienkos. 2018. "Enhanced biological fixation of methane for microbial lipid production by recombinant *Methylobacterium buryatense*." *Biotechnology for Biofuels* 11, no. 129: 1-11. <https://doi.org/10.1186/s13068-018-1128-6>.
161. Henard, C.A., and M.T. Guarnieri. 2016. "Metabolic and techno-economic assessment of high-potential hydrocarbon targets from methane, down-selecting two targets for FY17 efforts." NREL Milestone Report.
162. Anderson, Eric M., Rui Katahira, Michelle Reed, Michael G. Resch, Eric M. Karp, Gregg T. Beckham, and Yuriy Román-Leshkov. 2016. "Reductive catalytic fractionation of corn stover lignin." *ACS Sustainable Chemistry & Engineering* 4, no. 12: 6940–6950. <https://doi.org/10.1021/acssuschemeng.6b01858>.
163. Anderson, Eric M., Michael L. Stone, Rui Katahira, Michelle Reed, Gregg T. Beckham, and Yuriy Román-Leshkov. 2017. "Flowthrough Reductive Catalytic Fractionation of Biomass." *Joule* 1, no. 3: 613–622. <https://doi.org/10.1016/j.joule.2017.10.004>.
164. Laskar, Dhrubojyoti D., Melvin P. Tucker, Xiaowen Chen, Gregory L. Helms, and Bin Yang. 2014. "Noble-metal catalyzed hydrodeoxygenation of biomass-derived lignin to aromatic hydrocarbons." *Green Chemistry* 16, no. 2: 897–910. <https://doi.org/10.1039/C3GC42041H>.
165. Agile BioFoundry. 2018. "Agile BioFoundry Home Page." <https://agilebiofoundry.org/>.

Appendix A. Individual Equipment Costs Summary

The following table shows abbreviated specifications, purchased cost, and installed cost for each piece of equipment in this process design. Although each piece of equipment has its own line, many were quoted as part of a package, so their scaling calculations are not shown. NREL would like to acknowledge the subcontractors and equipment vendors who assisted us with cost estimates over recent years as were utilized for this design report.

Acids Pathway

A200: Pretreatment		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Flash Tank Agitator	Side-mounted, 3 x 75 hp. (170 kW)	170 kW	316LSS	3	\$90,000	2009	\$90,000	strm.a200.254	252891	kg/hr	0.50	1.5	192,146	0.76	\$78,450	\$81,426	\$122,139
Ammonia Addition Tank Agitator		10 hp	SS	1	\$21,900	2009	\$21,900	strm.a200.228	410369	kg/hr	0.50	1.5	230,647	0.56	\$16,418	\$17,041	\$25,562
Ammonia Static Mixer			SS	1	\$5,000	2009	\$5,000	strm.a200.275	157478	kg/hr	0.50	1.0	38,500	0.2445	\$2,472	\$2,566	\$2,566
Pretreatment Water Heater	29.9 MMBtu		304SS	1	\$92,000	2010	\$92,000	Heat.A200.QH201	-8	Gcal/hr	0.70	2.2	(0.29)	0.04	\$9,453	\$9,297	\$20,453
Pretreatment Sugar Beet extruder				1	\$5,424,000	2010	\$5,424,000	SCIS.a200.DEAC-IN	38600	kg/hr	1.00	1.0	70,483	1.83	\$9,904,187	\$9,740,555	\$9,740,555
Milling Equipment	200kw/dry ton			8	\$2,466,700	2013	\$2,466,700	SCIS.a200.211b	62942	kg/hr	0.60	1.5	57,306	0.91	\$19,733,600	\$18,843,101	\$28,264,651
Milling Equipment-Szego Mill				11	\$578,000	2013	\$578,000	SCIS.a200.211b	62942	kg/hr	0.60	1.4	57,306	0.91	\$6,358,000	\$6,071,089	\$8,499,524
Blowdown Tank Discharge Pump	1900 GPM, 150 FT TDH	125	316SS	1	\$25,635	2010	\$25,635	strm.a200.222	292407	kg/hr	0.80	2.3	193,144	0.66	\$18,397	\$18,093	\$41,614
Flash Tank Discharge Pump	900 GPM, 150 FT TDH	75	316SS	1	\$30,000	2009	\$30,000	strm.a200.254	204390	kg/hr	0.80	2.3	192,146	0.94	\$28,554	\$29,637	\$68,165
Deacetylation Tank Discharge Pump	1771 GPM, 150 FT TDH	100	316SS	1	\$22,500	2009	\$22,500	strm.a200.211a	402194	kg/hr	0.80	2.3	283,665	0.71	\$17,017	\$17,662	\$40,624
Hydrolyzate Pump	1771 GPM, 150 FT TDH	100	316SS	1	\$22,500	2009	\$22,500	strm.a200.228	402194	kg/hr	0.80	2.3	230,647	0.57	\$14,421	\$14,968	\$34,426
Deacetylation reactor conveyors	Feed and discharge drag conveyors	40 hp	SS316	3	\$110,000	2013	\$110,000	strm.a200.211a	277167	kg/hr	0.80	1.7	283,665	1.02	\$336,175	\$321,004	\$545,707
S/L Split Discharge Pump to WWT	900 GPM, 150 FT TDH	75	316SS	1	\$30,000	2009	\$30,000	strm.a200.4	204390	kg/hr	0.80	2.3	193,144	0.94	\$28,672	\$29,760	\$68,447
Flash Tank	23' x 48' - 110,000 gal.		SS316	1	\$511,000	2009	\$511,000	strm.a200.223	264116	kg/hr	0.70	2.0	193,144	0.73	\$410,470	\$426,042	\$852,084
Ammonia Addition Tank	118,000 gal, 1hr residence time		SS304	1	\$236,000	2009	\$236,000	strm.a200.228	410369	kg/hr	0.70	2.0	230,647	0.56	\$157,671	\$163,653	\$327,306
Area 200 Totals															\$37,113,956	\$35,785,895	\$48,653,825

A300: Hydrolysis and Fermentation		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Continuous Enzymatic Hydrolysis Bulk																	
Hydrolyzate Heater	Plate & Frame 32.5 MMBtu/hr		SS 304	1	\$85,000	2010	\$85,000	heat.A300.CEH.QC301	-8	Gcal/hr	0.70	2.2	(8)	0.9910	\$84,461	\$83,066	\$182,745
Reactor 1	Basis = 1,000,000 gallon ea		304SS	1	\$844,000	2009	\$844,000	Volume Flow	1000000	gal	1.00	1.5	2,350,067	2.35	\$1,983,457	\$2,058,706	\$3,088,059
Reactor 2	Basis = 1,000,000 gallon ea		304SS	1	\$844,000	2009	\$844,000	Volume Flow	1000000	gal	1.00	1.5	2,257,326	2.26	\$1,905,183	\$1,977,463	\$2,966,194
Reactor 3	Basis = 1,000,000 gallon ea		304SS	1	\$844,000	2009	\$844,000	Volume Flow	1000000	gal	1.00	1.5	2,087,882	2.09	\$1,762,172	\$1,829,026	\$2,743,539
CEH Cooler	Plate & frame		304SS	1	\$86,928	2009	\$86,928	one per reactor	12	ea	1.00	2.2	3	0.25	\$21,732	\$22,556	\$49,624
CEH recirculation pump	340 GPM, 150 FT	20.0	316SS	1	\$47,200	2009	\$47,200	one per reactor	12	ea	0.80	2.3	3	0.25	\$15,570	\$16,161	\$37,170
CEH MF membranes	Ultrafiltration- scaled from Nexant value			1	\$2,048,000	2011	\$2,048,000	area required	53820	ft ² /unit	1.00	2.5	95,783	1.78	\$3,644,804	\$3,370,993	\$8,427,482
CEH UF membranes	Ultrafiltration- scaled from Nexant value			1	\$2,048,000	2011	\$2,048,000	area required	53820	ft ² /unit	1.00	2.5	114,939	2.14	\$4,373,765	\$4,045,191	\$10,112,978
CEH membrane spare	Ultrafiltration- scaled from Nexant value			1	\$2,048,000	2011	\$2,048,000	units	53820	ft ² /unit	1.00	2.5	31,928	0.59	\$1,214,935	\$1,123,664	\$2,809,161
Lignin Press	From EtOH model lignin press + supporting equip		316SS	2	\$3,294,700	2010	\$3,294,700	strm.A300.CEH.LPRESS.571	31815	kg/hr	0.80	1.7	22,221	0.70	\$2,472,386	\$2,431,538	\$4,133,615
Sugar Concentration		3600 kW	304SS	1	\$6,370,000	2013	\$6,370,000	strm.A300.EVAP.301SUG	244084	kg/hr	0.70	2.0	788,352	3.23	\$14,473,253	\$13,820,133	\$27,640,265
Concentrated Sugar Storage Tank	5,500 gallons - 20 min residence time	20 hp	SS	1	\$168,000	2011	\$168,000	strm.A300.SUG-EVAP	76712	kg/hr	0.70	1.8	179,172	2.34	\$304,225	\$381,370	\$506,467
Area 300 Totals															\$32,255,943	\$31,059,867	\$62,697,299

A400:Enzyme Production		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Cellulase Fermentor Agitators		800.0	SS316		\$580,000	2009	\$580,000	CLVESSEL		1 ea	1.00	1.5	5	5.00	\$2,900,000	\$3,010,021	\$4,515,032
Cellulase Fermentor Agitators		0.75hp	SS316		\$3,420	2009	\$3,420	ICLSEED		1 ea	1.00	1.5	4	4.00	\$13,680	\$14,199	\$21,298
Cellulase Fermentor Agitators		8 hp	SS316		\$11,000	2009	\$11,000	ICLSEED		1 ea	1.00	1.5	4	4.00	\$44,000	\$45,669	\$68,504
Cellulase Fermentor Agitators		80 hp	SS316		\$63,000	2009	\$63,000	ICLSEED		1 ea	1.00	1.5	4	4.00	\$252,000	\$261,560	\$392,341
Cellulase Nutrient Mix Tank Agitator		3 hp	CS	1	\$4,800	2009	\$4,800	strm.a400.416	174	kg/hr	0.50	1.6	123	0.70	\$4,030	\$4,182	\$6,692
Cellulase Hold Tank Agitator		10 hp	SS316	1	\$26,900	2009	\$26,900	strm.422	10930	kg/hr	0.50	1.5	7,575	0.69	\$22,395	\$23,244	\$34,866
Cellulase Fermentor	80,000 gal, 1 atm, 28 °C, Internal coil		SS316		\$400,500	2009	\$400,500	CLVESSEL		1 ea	1.00	2.0	5	5.00	\$2,002,500	\$2,078,471	\$4,156,943
1st Cellulase Seed Fermentor	80 gallon skid complete - \$46,000 ea		304SS		\$46,000	2009	\$46,000	ICLSEED		1 ea	1.00	1.8	4	4.00	\$184,000	\$190,981	\$343,765
2nd Cellulase Seed Fermentor	800 gallon skid complete - \$57,500 ea		304SS		\$57,500	2009	\$57,500	ICLSEED		1 ea	1.00	1.8	4	4.00	\$230,000	\$238,726	\$429,706
3rd Cellulase Seed Fermentor	8,000 gallon skid complete - \$95,400 ea		304SS		\$95,400	2009	\$95,400	ICLSEED		1 ea	1.00	1.8	4	4.00	\$381,600	\$396,077	\$712,939
Fermentor Air Compressor Package	8000 SCFM @ 16 psig		CS	2	\$350,000	2009	\$350,000	strm.a400.450	33168	kg/hr	0.60	1.6	17,839	0.54	\$241,242	\$250,395	\$400,632
Cellulase Transfer Pump	59 gpm, 100 FT, TDH SIZE 2X1-10C	3	316SS	1	\$7,357	2010	\$7,357	strm.a400.420	13399	kg/hr	0.80	2.3	7,575	0.57	\$4,662	\$4,585	\$10,545
Cellulase Seed Pump	3 GPM, 100 FT TDH SIZE 2X1-10	2	316SS	4	\$29,972	2010	\$29,972	strm.a400.409	681	kg/hr	0.80	2.3	421	0.62	\$20,408	\$20,071	\$46,163
Cellulase Nutrient Transfer Pump	Gear Pump 2 GPM, 100 FT	1	316SS	1	\$1,500	2009	\$1,500	strm.a400.416	454	kg/hr	0.80	2.3	123	0.27	\$526	\$546	\$1,257
Cellulase Feed Pump	Gear Pump	1	316SS	1	\$5,700	2009	\$5,700	strm.a400.422	18168	kg/hr	0.80	2.3	7,575	0.42	\$2,831	\$2,938	\$6,759
Anti-foam Pump	Gear Pump 2 GPM, 100 FT	1	316SS	1	\$1,500	2009	\$1,500	strm.a400.444	11	kg/hr	0.80	2.3	7	0.69	\$1,115	\$1,157	\$2,661
Cellulase Nutrient Mix Tank	HDPE, 8,000 gal		HDPE	1	\$9,000	2010	\$9,000	strm.a400.416	224	kg/hr	0.70	3.0	123	0.55	\$5,903	\$5,806	\$17,411
Cellulase Hold Tank	80,000 gal		304SS	1	\$248,070	2009	\$248,070	strm.a400.422	10930	kg/hr	0.70	1.8	7,575	0.69	\$191,921	\$199,202	\$358,564
Area 400 Totals															\$6,502,813	\$6,747,832	\$11,526,084

A500: Bioconversion & Upgrading		Mechanical Equipment List					Scaled Installed Costs												
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year		
C4 Acids Anaerobic Fermentation																			
Fermentor Feed Cooler	Plate & frame		SS304	1	\$23,900	2009	\$23,900	heat.A500.C4ACID.QC310		5 Gcal/hr	0.70	1.8	3	0.50	\$14,638	\$15,194	\$27,349		
Seed Hold Tank Agitator		15 hp	SS304	1	\$31,800	2009	\$31,800	STRM.A500.C4ACID.304	40414	kg/hr	0.50	1.5	15,918	0.39	\$19,957	\$20,714	\$31,071		
4th Seed Vessel Agitator		7.5 hp	SS	2	\$26,000	2009	\$26,000	NSDC4		2 ea	0.50	1.5	2	1.00	\$26,000	\$26,986	\$40,480		
5th Seed Vessel Agitator		10 hp	SS	2	\$43,000	2009	\$43,000	NSDC4		2 ea	0.50	1.5	2	1.00	\$43,000	\$44,631	\$66,947		
Beer Surge Tank Agitator		20 hp	SS304	2	\$68,300	2009	\$68,300	strm.PRD-500	425878	kg/hr	0.50	1.5	11,465	0.03	\$11,207	\$11,632	\$17,448		
1st Seed Fermentor	20 gallon skid complete - \$37,700 ea		3045S	2	\$75,400	2009	\$75,400	NSDC4		2 ea	0.70	1.8	2	1.00	\$75,400	\$78,261	\$140,869		
2nd Seed Fermentor	200 gallon skid complete - \$58,300 ea		3045S	2	\$116,600	2009	\$116,600	NSDC4		2 ea	0.70	1.8	2	1.00	\$116,600	\$121,024	\$217,842		
3rd Seed Fermentor	2000 gallon skid complete - \$78,800 ea		3045S	2	\$157,600	2009	\$157,600	NSDC4		2 ea	0.70	1.8	2	1.00	\$157,600	\$163,579	\$294,442		
4th Seed Fermentor	20,000 gallon, incl. coil - \$176,000 ea		3045S	2	\$352,000	2009	\$352,000	NSDC4		2 ea	0.70	2.0	2	1.00	\$352,000	\$365,354	\$730,709		
4th Seed Fermentor Coil	incl. w/ tank		3045S	1	INCLUDED														
5th Seed Fermentor	200,000 gallon, incl. coil - \$590,000 ea		3045S	2	\$1,180,000	2009	\$1,180,000	NSDC4		2 ea	0.70	2.0	2	1.00	\$1,180,000	\$1,224,767	\$2,449,534		
5th Seed Fermentor Coil	incl. w/ tank		3045S	1	INCLUDED														
Seed Hold Transfer Pump	190 GPM, 150 FT TDH	10	3165S	1	\$8,200	2009	\$8,200	STRM.A500.C4ACID.304	43149	kg/hr	0.80	2.3	15,918	0.37	\$3,693	\$3,833	\$8,815		
Seed Hold Tank	300,000 gallon		3165S	1	\$439,000	2009	\$439,000	STRM.A500.C4ACID.304	40414	kg/hr	0.70	1.8	15,918	0.39	\$228,668	\$237,343	\$427,217		
Seed Transfer Pump	190 GPM, 615 FT TDH	40	3165S	2	\$24,300	2009	\$24,300	STRM.A500.C4ACID.304	43149	kg/hr	0.80	2.3	15,918	0.37	\$10,943	\$11,358	\$26,123		
Fermentor Tank (Anaerobic)			3045S	12	\$10,128,000	2009	\$10,128,000	NVESC4		12 ea	1.00	1.5	3	0.25	\$2,532,000	\$2,628,060	\$3,942,090		
Fermentor Agitator		30 hp	SS304	1	\$52,500	2009	\$52,500	NVESC4		1 ea	1.00	1.5	3	3.00	\$157,500	\$163,475	\$245,213		
Fermentation Cooler	Plate & frame		3045S	12	\$86,928	2009	\$86,928	NVESC4		12 ea	1.00	2.2	3	0.25	\$21,732	\$22,556	\$49,624		
Fermentation Recirc/Transfer Pump	340 GPM, 150 FT	20	3165S	5	\$47,200	2009	\$47,200	NVESC4		12 ea	0.80	2.3	3	0.25	\$15,570	\$16,161	\$37,170		
PSA Fermentation Vent					\$975,000	2013	\$975,000	strm.A500.C4ACID.FERM-VNT	13528	kg/hr	0.60	1.9	23,057	1.70	\$1,342,604	\$1,282,018	\$2,435,834		
Bioreactor Transfer Pump	2152 GPM, 171 FT TDH	125	3165S	1	\$26,800	2009	\$26,800	strm.PRD-500	488719	kg/hr	0.80	2.3	11,465	0.02	\$1,332	\$1,382	\$3,179		
Bioreactor Storage Tank	1,200,000 gallon		3165S	1	\$1,317,325	2011	\$1,317,325	strm.PRD-500	156789	kg/hr	0.70	1.8	11,465	0.07	\$211,128	\$195,268	\$351,482		
C4 Recovery and Upgrading																			
Feed Pump				2	\$9,200	2009	\$9,200	STRM.A500.C4ACID.AQIN		26881	kg/hr	0.80	3.1	157,613	6.95	\$43,384	\$45,030	\$139,593	
Separations (LPME)				1	\$8,000,000	2010	\$8,000,000	STRM.A500.C4ACID.6	362200	kg/hr	0.70	2.0	173,644	0.48	\$4,781,768	\$4,702,766	\$9,405,532		
Extraction Economizer	IF calculated in HP column	654,100			\$376,500	2015	\$376,500	HEAT.A500.C4ACID.QX-ORG1	2.48	Gcal/hr	1.00	1.7	2	1.00	\$376,492	\$366,282	\$636,348		
Extraction Vacuum Tower	IF calculated in HP column	924,000			\$353,700	2015	\$353,700	STRM.A500.C4ACID.FD-FORG	38594.00	kg/hr	1.00	2.6	37,107	0.96	\$340,071	\$330,849	\$864,304		
Condensor	IF calculated in HP column	62,000			\$11,000	2015	\$11,000	HEAT.A500.C4ACID.QC-FORG	1.31	Gcal/hr	1.00	5.6	1	0.95	\$10,451	\$10,167	\$57,306		
Condensor accumulator	IF calculated in HP column	109,200			\$17,100	2015	\$17,100	HEAT.A500.C4ACID.QC-FORG	1.31	Gcal/hr	1.00	6.4	1	0.95	\$16,246	\$15,805	\$100,932		
Reboiler	IF calculated in HP column	329,900			\$217,000	2015	\$217,000	HEAT.A500.C4ACID.QHP-FORG	-1.51	Gcal/hr	1.00	1.5	(2)	1.00	\$216,413	\$210,544	\$320,086		
Reflux pump	IF calculated in HP column	39,100			\$5,800	2015	\$5,800	HEAT.A500.C4ACID.QC-FORG	1.31	Gcal/hr	1.00	6.7	1	0.95	\$5,510	\$5,361	\$36,140		
RXR1 Feed Pump				2	\$9,200	2009	\$9,200	STRM.A500.C4ACID.AQIN		26881	kg/hr	0.80	3.1	157,613	6.95	\$43,384	\$45,030	\$139,593	
RXR1 preheat			SS304	1	\$41,000	2009	\$41,000	HEAT.A500.C4ACID.32	-2	Gcal/hr	0.70	2.2	(1)	0.27	\$16,598	\$17,228	\$37,901		
RXR 1 (Ketone/ization)				1	\$2,044,000	2014	\$2,044,000	STRM.A500.C4ACID.16	53204	kg/hr	0.37	2.2	21,075	0.40	\$1,451,036	\$1,364,392	\$3,001,662		
RXR1 Economizer	IF calculated in HP column	447,300			\$251,000	2015	\$251,000	HEAT.A500.C4ACID.QX-KETO	1.75	Gcal/hr	1.00	1.8	1	0.76	\$251,000	\$244,193	\$435,170		
RXR condensor				1	\$487,000	2010	\$487,000	HEAT.A500.C4ACID.31	23	Gcal/hr	0.60	2.8	2	0.08	\$108,327	\$106,537	\$298,303		
RXR1 Condensor	IF calculated in HP column	112,700			\$26,200	2015	\$26,200	HEAT.A500.C4ACID.31	3.36	Gcal/hr	1.00	4.3	2	0.56	\$14,782	\$14,381	\$61,859		
RXR1 2 Phase Flash	IF calculated in HP column	127,700			\$22,500	2015	\$22,500	STRM.A500.C4ACID.FD1-FLSH	22563	kg/hr	1.00	5.7	21,075	0.93	\$21,017	\$20,447	\$116,046		
RXR1 Vent Scrubber	Inlet Gas: 9681 acfm, 91°F, 1.97 mass% Ethanol		SS304/PP		\$215,000	2009	\$215,000	STRM.A500.C4ACID.SCRB-FD1	22608.00	kg/hr	0.60	2.4	9,704	0.43	\$129,431	\$134,342	\$322,420		
RXR1 Scrubber Bottoms Pump	108 GPM, 104 FT TDH		3165S	1	\$6,300	2009	\$6,300	STRM.A500.C4ACID.SCRB-BTM	24527.00	kg/hr	0.80	2.3	145,930	5.95	\$26,239	\$27,234	\$62,638		
RXR1 Decanter	(4) 9,841 gallon vessels		3045S	4	\$588,000	2013	\$588,000	STRM.A500.C4ACID.FD1-S1	156789	kg/hr	0.50	2.0	145,930	0.93	\$567,272	\$541,673	\$1,083,346		
RXR2 Feed Pump	IF calculated in HP column	124,400			\$52,200	2015	\$52,200	STRM.A500.C4ACID.FD-RMIX	237365	kg/hr	1.00	2.4	101,236	0.43	\$22,263	\$21,660	\$51,618		
RXR2 preheat	IF calculated in HP column	301,500			\$142,600	2015	\$142,600	HEAT.A500.C4ACID.QH-RCOND	-5.86	Gcal/hr	1.00	2.1	(1)	0.14	\$19,544	\$19,014	\$40,200		
CSTR ketone condensation (5hr residence time scaling (redo in ACCE eventually))	IF calculated in HP column	3,601,400			\$1,993,000	2015	\$1,993,000	STRM.A500.C4ACID.22	237365.42	kg/hr	1.00	1.8	303,709	1.28	\$2,550,041	\$2,480,885	\$4,483,021		
					SIZING			Residence time		15.00	hr								
CSTR Agitator	from anaerobic fermentor quote	30 hp	SS304	1	\$52,500	2009	\$52,500	STRM.A500.C4ACID.22	237365.42	ea	1.00	1.5	101,236	0.43	\$22,391	\$23,241	\$34,861		
RXR2 HHPs	IF calculated in HP column	296,900			\$85,800	2015	\$85,800	STRM.A500.C4ACID.11	237365.42	kg/hr	1.00	3.5	101,236	0.43	\$36,594	\$35,601	\$123,194		
RXR Catalyst Filter(scroll discharge centrifuge)	IF calculated in HP column	100,700			\$79,700	2015	\$79,700	STRM.A500.C4ACID.H2O-CAT	4464	kg/hr	1.00	1.3	1,055	0.24	\$18,831	\$18,320	\$23,148		
Ketone Recycle Tower	IF calculated in HP column	943,600			\$286,000	2015	\$286,000	STRM.A500.C4ACID.FRAC-FD	232901.00	kg/hr	1.00	3.3	100,181	0.43	\$123,021	\$119,684	\$394,875		
Condensor	IF calculated in HP column	78,200			\$16,400	2015	\$16,400	HEAT.A500.C4ACID.QC-FRAC	5.83	Gcal/hr	1.00	4.8	5	0.86	\$14,138	\$13,755	\$65,588		
Condensor accumulator	IF calculated in HP column	165,200			\$32,600	2015	\$32,600	HEAT.A500.C4ACID.QC-FRAC	5.83	Gcal/hr	1.00	5.1	5	0.86	\$28,104	\$27,342	\$138,556		
Reboiler	IF calculated in HP column	721,600			\$318,800	2015	\$318,800	HEAT.A500.C4ACID.QHP-FRAC	-19.61	Gcal/hr	1.00	2.3	(5)	0.25	\$79,525	\$77,368	\$175,122		
Reflux pump	IF calculated in HP column	71,700			\$13,100	2015	\$13,100	HEAT.A500.C4ACID.QC-FRAC	5.83	Gcal/hr	1.00	5.5	5	0.86	\$11,293	\$10,987	\$60,136		
Furnace				1	\$241,400	2011	\$241,400	HEAT.A500.C4ACID.QOIL	-2.4187	MMkcal/	0.70	1.5	(8)	3.30	\$557,190	\$515,332	\$783,305		
C4 HDO																			
HDO Feed Pump	IF calculated in HP column	420,200			\$201,600	2015	\$201,600	STRM.A500.C4ACID.TO-HDO	221115	kg/hr	1.00	2.1	12,137	0.05	\$11,066	\$10,766	\$22,440		
HDO feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	STRM.A500.C4ACID.FRAC-BTM	290932	kg/hr	0.60	2.50	12,137	0.04	\$6,833	\$6,320	\$15,800		
HDO reactor pump					\$802,861	2014	\$802,861	STRM.A500.C4ACID.FRAC-BTM	208720	kg/hr	0.80	1.40	12,137	0.06	\$82,469	\$77,544	\$108,562		
HDO trim preheater			3045S		\$41,000	2009	\$41,000	HEAT.A500.C4ACID.QX-BTM	-2	MMkcal/	0.70	2.20	1	0.34	\$19,117	\$19,842	\$43,653		
HDO Fixed Bed Reactor	(Q3 FY17 milestone), base PF=2.5, 208 BBL/hr (>1000PSIG=2.5, 900=2.3, 800=1.9, 700=1.8, 600=1.6, 500=1.45, 400=1.35)			1.6	\$4,168,568	2011	\$4,168,568	Volume Flow (liquid)	32895	L/hr	0.70	2.00	13,258	0.40	\$2,206,593	\$2,040,825	\$4,081,651		
Pressure Follower (via Guthrie)								strm.A500.C4ACID.HDO-LIQ	29274	kg/hr			12,137						
Internals								den.A500.C4ACID.HDO-LIQ		1	GM/CC								
HDO Effluent economizer	2-4 TEMA shell and tube HX		3165S		\$353,600	2011	\$353,600	HEAT.A500.C4ACID.QX-HDO	14	MMkcal/	0.70	2.66	3	0.19	\$110,628	\$102,317	\$271,737		
H2 Makeup Compressor	recipricating compressor(5 stages)				\$1,621,200	2011	\$1,621,200	strm.A500.C4ACID.H2-MU	390	kg/hr	0.60	1.09	412	1.06	\$1,675,703	\$1,549,818	\$1,6		

A600: WWT		Mechanical Equipment List				Scaled Installed Costs											
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Aeration Basin	Concrete and steel, not installed cost		Concrete	3	\$4,804,854	2012	\$4,804,854	Hydraulic flow	2.7	MGD	0.60	2.1	3	1.05	\$4,933,464	\$4,571,429	\$9,462,858
Pump - Centrifugal, Aeration Basin Feed	852 gpm ea	45 hp	CS	4	\$64,800	2012											
Aeration Grid	Full floor aeration grid		CS	1	\$2,500,000	2012											
Caustic Feed System		1.5 hp	CS	4	\$20,000	2012	\$20,000	COD	5600	kg/hr	0.60	3.0	4,149	0.74	\$16,706	\$15,480	\$46,440
Blowers	15000 SCFM @ 10.3psig ea	1000 hp ea	CS	9	\$2,070,000	2012	\$2,070,000	COD	5600	kg/hr	0.60	2.0	4,149	0.74	\$1,729,052	\$1,602,168	\$3,204,336
Membrane Bioreactor	Includes membrane, CIP, Scour system	85 hp ea	CS	1	\$4,898,500	2012	\$4,898,500	Hydraulic flow	2.7	MGD	1.00	1.6	3	1.05	\$5,118,971	\$4,743,323	\$7,779,050
Pump, Centrifugal, MBR, RAS		160 hp	CS	6	INCLUDED	2012											
Gravity Belt Thickeners	2m presses	48hp	CS	3	\$750,000	2012	\$750,000	COD	5600	kg/hr	0.60	1.6	4,149	0.74	\$626,468	\$580,496	\$922,988
Centrifuge		165 hp ea	CS	1	\$686,800	2012	\$686,800	COD	5600	kg/hr	0.60	2.7	4,149	0.74	\$573,678	\$531,579	\$1,429,948
Pump, Centrifugal, Centrifuge Feed	105 gpm	15hp	CS	2	INCLUDED	2012											
Pump, Submersible, Centrate	100 gpm	10 hp ea	CS	2	INCLUDED	2012											
Dewatering Polymer Addition	9.8 gph neat polymer	1 hp ea	CS	2	INCLUDED	2012											
Conveyor		10 hp ea	CS	1	\$7,000	2012	\$7,000	COD	5600	kg/hr	0.60	2.9	4,149	0.74	\$5,847	\$5,418	\$15,495
Reverse Osmosis			CS	7	\$2,450,000	2012	\$2,450,000	Hydraulic flow	2.7	MGD	1.00	1.8	3	1.05	\$2,560,269	\$2,372,388	\$4,151,679
Evaporator	368 gpm	1480 hp ea	Titanium	1	\$5,000,000	2012	\$5,000,000	Hydraulic flow	2.7	MGD	0.60	1.6	3	1.05	\$5,133,833	\$4,757,094	\$7,658,922
Ammonia Addition System	0.63 gpm	4.5 hp	CS	4	\$195,200	2012	\$195,200	COD	5600	kg/hr	0.60	1.5	4,149	0.74	\$163,049	\$151,084	\$232,669
Sodium Sulfate Purification																	
Evaporator feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	strm.A600.23	290932	kg/hr	0.60	2.50	278,983	0.96	\$44,824	41456.46261	\$103,641
Evaporator feed heater	shell and tube 1/2 pass				\$274,818	2011	\$274,818	heat.A600.31	-13	MMkcal/	0.60	3.00	(5)	0.35	\$146,548	135538.527	\$406,616
Evaporator flash drum	23' x 48' - 110,000 gal.		SS316	1	\$511,000	2009	\$511,000	strm.A600.23	264116	kg/hr	0.70	2.00	278,983	1.06	\$530,969	551113.1278	\$1,102,226
Centrifuge	Nexant quote sodium sulfate, 25410 lb/hr solids basis			1	\$327,680	2011	\$327,680	strm.A600.NA2504	11524	kg/hr	0.60	2.3	14,565	1.26	\$377,117	\$348,786	\$802,209
Dryer	Nexant quote Sodium sulfate, 25410 lb/hr solids basis			1	\$555,008	2011	\$555,008	strm.A600.PRD-SALT	11524	kg/hr	0.60	2.6	13,871	1.20	\$620,314	\$573,714	\$1,491,656
Area 600 Totals															\$22,581,108	\$20,981,066	\$38,810,731

A700: Lignin Utilization		Mechanical Equipment List				Scaled Installed Costs												
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year	
A701: Lignin Conditioning																		
Neutralization Tank	2.6 atm, 130C operating @ 30 min. hold = 30,000 gal		SS317	1	\$236,000	2009	\$236,000	strm.A700.A701.LIQUID1	410369	kg/hr	0.70	2.0	86,005	0.21	\$79,041	\$82,040	\$164,080	
Pulping Reactor Tank	2.6 atm, 130C operating (up to 160C, 30 min.) @ 30,000 gal		SS316	1	\$16,300,000	2013	\$16,300,000	strm.A700.A701.PULP-OUT	323295	kg/hr	0.60	1.7	115,134	0.36	\$8,773,033	\$8,377,141	\$13,822,282	
Flash/drain tank			SS317	1	\$262,000	2013	\$262,000	strm.A700.A701.PULP-OUT	323296	kg/hr	0.70	2.0	115,134	0.36	\$127,181	\$121,442	\$242,884	
Black Liquor Storage Tank	1,200,000 gallon		316SS	1	\$1,317,325	2011	\$1,317,325	strm.A700.A701.5	328984	kg/hr	0.70	1.8	92,912	0.28	\$543,652	\$502,811	\$905,059	
A702: Muconate Fermentation																		
1st Aerobic Seed	80 gallon skid complete - \$46,000 ea		304SS		\$46,000	2009	\$46,000	NSD1000		1 ea	1.00	1.80	3	3.00	\$138,000	\$143,235	\$257,824	
1st Seed Vessel Agitator		0.75hp	SS316		\$3,420	2009	\$3,420	NSD1000		1 ea	1.00	1.50	3	3.00	\$10,260	\$10,649	\$15,974	
2nd Aerobic Seed	800 gallon skid complete - \$57,500 ea		304SS		\$57,500	2009	\$57,500	NSD1000		1 ea	1.00	1.80	3	3.00	\$172,500	\$179,044	\$322,280	
2nd Seed Vessel Agitator		8 hp	SS316		\$11,000	2009	\$11,000	NSD1000		1 ea	1.00	1.50	3	3.00	\$33,000	\$34,252	\$51,378	
Bubble column seed fermentor	100 m3		316SS		\$274,100	2014	\$274,100	NSD1000		1 ea	1.00	2.30	3	3.00	\$822,300	\$773,199	\$1,778,358	
Seed circulation cooler	650 sqft		316SS		\$8,400	2014	\$8,400	NSD1000		1 ea	1.00	2.20	3	3.00	\$25,200	\$23,695	\$52,130	
Bubble column production fermentor	1000 m3		316SS		\$1,691,400	2014	\$1,691,400	NVES1000		1 ea	1.00	2.30	17	17.00	\$28,753,800	\$27,036,857	\$62,184,772	
Production circulation cooler	4500 sqft		316SS		\$48,100	2014	\$48,100	NVES1000		1 ea	1.00	2.20	17	17.00	\$817,700	\$768,874	\$1,691,522	
Production circulation pump	400 gpm		316SS		\$11,500	2014	\$11,500	NVES1000		1 ea	1.00	2.30	17	17.00	\$195,500	\$183,826	\$422,801	
Fermentation air compressor	25,000 ACFM @ 45psig; max size in ACCE		CS		\$1,318,600	2014	\$1,318,600	AIRV1000		13 m ³ /s	1.00	1.60	15	1.11	\$1,464,541	\$1,377,090	\$2,203,345	
Fermentation air receiver	25,000 gal		CS		\$104,600	2014	\$104,600	AIRV1000		13 m ³ /s	1.00	2.00	15	1.11	\$116,177	\$109,240	\$218,480	
Fermentation Surge tank	insulated cone bottom, 6460 gal				\$45,966	2011	\$45,966	strm.A700.A702.UF-FD	290932	kg/hr	0.60	2.50	164,564	0.57	\$32,656	\$30,203	\$75,507	
Ultrafiltration membrane separator					\$2,048,000	2011	\$2,048,000	Volume Flow	1303	GPM	0.60	2.50	711	1.00	\$2,048,000	\$1,894,146	\$4,735,366	
membrane broth feed pump					INCLUDED			strm.A700.A702.UF-FD		kg/hr			164,564					
membrane solvent feed pump					INCLUDED			den.A700.A702.UF-FD		gm/cc			1					
A703: Recovery and Upgrading																		
Carbon Filter	2 Vessels, for color removal				\$345,234	2011	\$345,234	Volume Flow	1347	GPM	0.60	2.50	657	1.00	\$345,234	319298.7157	\$798,247	
Initial carbon loading					INCLUDED	2011		strm.A700.A703.CFIL-FD		kg/hr			151,994					
								den.A700.A703.CFIL-FD		gm/cc			1					
CCM Crystallizer	Oslo Type. 2 In series		316SS	2 series	\$7,104,192	2011	\$7,104,192	Volume Flow	190	GPM	0.60	2.50	39	0.21	\$2,757,128	2550001.932	\$6,375,005	
								strm.A700.A703.CRY1-PRD		kg/hr	0.60	2.50	11,164					
								den.A700.A703.CRY1-PRD		g/cc	0.60	2.50	1					
CCM Centrifuge	Centrifuge Separator				\$327,680	2011	\$327,680	strm.A700.A703.CRY1-PRD	13403	kg/hr	0.60	2.30	11,164	0.83	\$293,642	271582.9452	\$624,641	
CCM Drier	Fluidized bed drier parallel			2 parallel	\$555,008	2011	\$555,008	strm.A700.A703.DRY1-PRD	11526	kg/hr	0.60	2.60	10,613	0.92	\$528,188	488508.7424	\$1,270,123	
Dissolution Tank	mixing tank to redissolve crystals in solvent (EtOH)				\$1,317,325	2011	\$1,317,325	strm.A700.A703.FIL2-FD	328984	kg/hr	0.70	1.80	52,507	0.16	\$364,606	337215.6969	\$606,988	
Dissolution Tank agitator	pump to retain crystal suspension	80	316SS		\$63,000	2009	\$63,000	work.A700.A703.W-ETOHMX	60	kW	1.00	1.50	60	1.00	\$63,000	65390.10165	\$98,085	
Filtration Centrifuge(salt removal)	removes precipitated solids after dissolution				\$327,680	2011	\$327,680	strm.A700.A703.FIL2-SLT	13403	kg/hr	0.60	2.30	145	0.01	\$21,686	20057.1257	\$46,131	
HDO feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	strm.A700.A703.FIL2-PRD	290932	kg/hr	0.60	2.50	52,362	0.18	\$16,428	15193.43013	\$37,984	
HDO reactor pump					\$802,861	2014	\$802,861	strm.A700.A703.FIL2-PRD	208720	kg/hr	0.80	1.40	52,362	0.25	\$265,585	249726.104	\$349,617	
HDO Feed Effluent economizer	2-4 TEMA shell and tube HX		316SS		\$353,600	2011	\$353,600	heat.A700.A703.QX-HDO	14	MmKcal/h	0.70	2.66	2	0.16	\$99,796	92298.92956	\$245,130	
HDO trim preheater			304SS		\$41,000	2009	\$41,000	heat.A700.A703.QH-TRIM	-2	MmKcal/h	0.70	2.20	-	0.00	\$0	0	\$0	
HDO Fixed Bed Reactor	(Q3 FY17 milestone), base PF=2.5, 208 BBL/hr				\$4,168,568	2011	\$4,168,568	Volume Flow (liquid)	32895	L/hr	0.70	2.00	64,618	1.96	\$6,687,190	6184823.24	\$12,369,646	
Pressure Factor (via Guthrie)	(>100PSIG=2.5, 900=2.3, 800=1.9, 700=1.8, 600=1.6, 500=1.45, 400=1.35)		1.6		INCLUDED			strm.A700.A703.RXR-FD	29274	kg/hr	0.70	2.00	52,362					
Internals					INCLUDED			den.A700.A703.RXR-FD		1 GM/CC			1					
Hydrogenation Intercooler (bed1)					\$2,353,181	2007	\$2,353,181	heat.A700.A703.QC-BED1	32	MmKcal/h	0.65	2.21	2	0.05	\$349,789	360640.6048	\$797,016	
Hydrogenation Intercooler (bed2)					\$2,353,181	2007	\$2,353,181	heat.A700.A703.QC-BED2	32	MmKcal/h	0.65	2.21	3	0.09	\$475,158	498999.3827	\$1,082,678	
H2 Makeup Compressor	reciprocating compressor(5 stages)				\$1,621,200	2011	\$1,621,200	strm.A700.A703.H2-MU	390	kg/hr	0.60	1.09	397	1.02	\$1,639,741	1516557.048	\$1,652,853	
H2 Makeup Compressor spare	reciprocating compressor(5 stages)				\$1,621,200	2011	\$1,621,200	strm.A700.A703.H2-MU	390	kg/hr	0.60	1.08	397	1.02	\$1,639,741	1516557.048	\$1,639,756	
HHPs	Via Adipic model(via MB)				\$436,000	2013	\$436,000	strm.A700.A703.HHPs-FD	119841	kg/hr	1.00	1.50	52,759	0.44	\$191,946	183284.4664	\$274,927	
HDO hot gas cooler					\$321,600	2011	\$321,600	heat.A700.A703.QAC-2	4	MmKcal/h	0.70	1.66	0	0.01	\$10,992	10166.28356	\$16,846	
CHPS	3-Phase horizontal sep., demister, 3/16 SS316 cladding				\$328,500	2011	\$328,500	Volume Flow	39911	L/hr	0.70	2.59	97	0.00	\$4,857	4492.299583	\$11,623	
PSA - Hydrogenation					\$975,000	2013	\$0	strm.A700.A703.CHPS-VAP	13528	kg/hr	0.60	1.90	104	0.01	\$0	0	\$0	
AA evaporator feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	strm.A700.A703.EVAP-FD	290932	kg/hr	0.60	2.50	92,707	0.32	\$23,144	21404.92784	\$53,512	
AA evaporator feed heater	shell and tube 1/2 pass				\$274,818	2011	\$274,818	heat.A700.A703.QH-EVAP	639	MmKcal/h	0.60	3.00	(2)	0.12	\$76,378	70639.95608	\$211,920	
AA evaporator flash drum	23' x 48' - 110,000 gal.		SS316	1	\$511,000	2009	\$511,000	strm.A700.A703.EVAP-FD	264116	kg/hr	0.70	2.00	92,707	0.35	\$245,552	254868.3281	\$509,737	
AA condenser drum					\$487,000	2010	\$487,000	heat.A700.A703.QC-COND	23	MmKcal/h	0.60	2.80	9	0.37	\$267,785	263360.6594	\$737,410	
AA Crystallizer	Oslo Type. 2 In series		316SS	2 series	\$7,104,192	2011	\$7,104,192	Volume Flow	190	GPM	0.60	2.50	42	0.22	\$2,857,243	2642595.854	\$6,806,490	
AA Centrifuge separator	Centrifuge Separator				\$327,680	2011	\$327,680	strm.A700.A703.CRY2-PRD	13403	kg/hr	0.60	2.30	11,336	0.85	\$296,355	274091.7995	\$630,411	
AA Drier	Fluidized bed drier parallel			2 parallel	\$555,008	2011	\$555,008	strm.A700.A703.DRY2-PRD	11526	kg/hr	0.60	2.60	10,798	0.94	\$533,697	493603.6734	\$1,283,370	
Totals:															\$64,207,402	\$60,344,005	\$127,474,183	

A800: CHP Mechanical Equipment List						Scaled Installed Costs											
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQ	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
High Solids Burner and Turbine																	
Burner Combustion Air Preheater	INCLUDED			1	INCLUDED												
BFW Preheater	INCLUDED			1	INCLUDED												
Pretreatment/BFW heat recovery	9.4 MM Btu/hr		SS304	1	\$41,000	2009	\$41,000	heat.A800.A810.QH812	-2	Gcal/hr	0.70	2.2	(2)	0.63	\$29,613	\$30,737	\$67,621
Air Intake Fan	INCLUDED				INCLUDED												
Boiler	525,000 lb/hr @ 900 psig		CS	1	\$28,550,000	2010	\$28,550,000	strm.A800.A810.813c	238203	kg/hr	0.60	1.8	141,781	0.60	\$20,912,586	\$20,567,081	\$37,020,745
Combustion Gas Baghouse	Baghouse, Spray dryer scrubber, flues/ducting			1	\$11,000,000	2013	\$0	strm.A800.A810.812	238203	kg/hr	0.60	1.8	126,623	0.53	\$0	\$0	\$0
Turbine/Generator	23.6 kW, 2 extractions			1	\$9,500,000	2010	\$9,500,000	work.A900.wtotal	-42200	kW	0.60	1.8	(20,318)	0.48	\$6,127,228	\$6,025,997	\$10,846,795
Hot Process Water Softener System				1	\$78,000	2010	\$78,000	strm.A800.A810.812	235803	kg/hr	0.60	1.8	126,623	0.54	\$53,712	\$52,825	\$95,084
Amine Addition Pkg.				1	\$40,000	2010	\$40,000	strm.A800.A810.812	235803	kg/hr	0.00	1.8	126,623	0.54	\$40,000	\$39,339	\$70,810
Ammonia Addition Pkg.				1	INCLUDED												
Phosphate Addition Pkg.				1	INCLUDED												
Condensate Pump			SS316	2	INCLUDED												
Turbine Condensate Pump			SS304	2	INCLUDED												
Deaerator Feed Pump			SS304	2	INCLUDED												
BFW Pump			SS316	5	INCLUDED												
Blowdown Pump			CS	2	INCLUDED												
Amine Transfer Pump			CS	1	INCLUDED												
Condensate Collection Tank			A285C	1	INCLUDED												
Condensate Surge Drum			SS304	1	INCLUDED												
Deaerator	Tray type		CS;SS316	1	\$305,000	2010	\$305,000	strm.A800.A810.812	235803	kg/hr	0.60	3.0	126,623	0.54	\$210,028	\$206,558	\$619,674
Area 800 Totals															\$27,373,167	\$26,922,537	\$48,720,730
A900: Utilities & Storage Mechanical Equipment List						Scaled Installed Costs											
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQ	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Utilities System																	
Cooling Tower System	44,200 gpm	750 hp	FIBERGLASS	1	\$1,375,000	2010	\$1,375,000	strm.a900.945	10037820	kg/hr	0.60	1.5	16,869,770	1.68	\$1,877,520	\$1,846,501	\$2,769,751
Plant Air Compressor	400 SCFM@125 psig	150 hp		1	\$28,000	2010	\$28,000	DRY101	83333	kg/hr	0.60	1.6	83,333	1.00	\$28,000	\$27,537	\$44,060
Chilled Water Package	2 x 2350 tons (14.2 MM kcal/hr)	3400 hp		1	\$1,275,750	2010	\$1,275,750	heat.a900.qchwp	14	Gcal/hr	0.60	1.6	49	3.47	\$2,689,031	\$2,644,604	\$4,231,366
CIP System	100,000 GAL		SS304/SS316	1	\$421,000	2009	\$421,000	strm.a900.914	63	kg/hr	0.60	1.8	145	2.30	\$694,222	\$720,560	\$1,297,008
Cooling Water Pump	16,120 GPM, 100 FT TDH SIZE 20X20-28	500.0	CS	3	\$283,671	2010	\$283,671	strm.a900.945	10982556	kg/hr	0.80	3.1	16,869,770	1.54	\$399,889	\$393,282	\$1,219,175
Make-up Water Pump	685 GPM, 75 FT TDH SIZE 6X4-13	20.0	CS	1	\$6,864	2010	\$6,864	strm.a900.904	155564	kg/hr	0.80	3.1	632,929	4.07	\$21,093	\$20,744	\$64,308
Process Water Circulating Pump	2285 GPM, 75 FT TDH SIZE 8X6-13	75.0	CS	1	\$15,292	2010	\$15,292	strm.a900.905	518924	kg/hr	0.80	3.1	1,334,219	2.57	\$32,551	\$32,013	\$99,241
Instrument Air Dryer	670 SCFM - CYCLING TYPE		CS	1	\$15,000	2009	\$15,000	DRY101	83333	kg/hr	0.60	1.8	83,333	1.00	\$15,000	\$15,569	\$28,024
Plant Air Receiver	3800 gal - 72" x 228" vertical		CS	1	\$16,000	2009	\$16,000	DRY101	83333	kg/hr	0.60	3.1	83,333	1.00	\$16,000	\$16,607	\$51,482
Process Water Tank No. 1	250,000 gal		CS	1	\$250,000	2009	\$250,000	strm.a900.905	451555	kg/hr	0.70	1.7	1,334,219	2.95	\$533,705	\$553,953	\$941,720
Storage																	
Ammonia Storage Tank	28,000 gal		SA- 516-70	2	\$196,000	2010	\$196,000	strm.A900.NH3-NET	1171	kg/hr	0.70	2.0	1,359	1.16	\$217,491	\$213,898	\$427,796
CSL Storage Tank	70,000 gal		Glass lined	1	\$70,000	2009	\$70,000	strm.A900.CSL-NET	1393	kg/hr	0.70	2.6	1,478	1.06	\$72,979	\$75,748	\$196,945
CSL Storage Tank Agitator		10 hp	SS304	1	\$21,200	2009	\$21,200	strm.A900.CSL-NET	1393	kg/hr	0.50	1.5	1,478	1.06	\$21,841	\$22,669	\$34,004
CSL Pump	8 GPM, 80 FT TDH	0.5	CS	1	\$3,000	2009	\$3,000	strm.A900.CSL-NET	1393	kg/hr	0.80	3.1	1,478	1.06	\$3,146	\$3,266	\$10,124
DAP Bulk Bag Unloader	Super sack unloader			1	\$30,000	2009	\$30,000	strm.A900.DAP-NET	163	kg/hr	0.60	1.7	714	4.38	\$72,754	\$75,515	\$128,375
DAP Bulk Bag Holder	Super sack holder			1	INCLUDED												
DAP Make-up Tank	12,800 gal		SS304	1	\$102,000	2009	\$102,000	strm.A900.DAP-NET	1615	kg/hr	0.70	1.8	714	0.44	\$57,580	\$59,765	\$107,576
DAP Make-up Tank Agitator		5.5 hp	SS304	1	\$9,800	2009	\$9,800	strm.A900.DAP-NET	163	kg/hr	0.50	1.5	714	4.38	\$20,504	\$21,282	\$31,923
DAP Pump	2 GPM, 100 FT TDH	0.5	CS	1	\$3,000	2009	\$3,000	strm.A900.DAP-NET	163	kg/hr	0.80	3.1	714	4.38	\$9,775	\$10,146	\$31,451
Sulfuric Acid Pump	5 GPM, 150 FT TDH SIZE 2X1-10	0.5	SS316	1	\$7,493	2010	\$7,493	strm.A900.ACID-NET	1981	kg/hr	0.80	2.3	10,531	5.32	\$28,518	\$28,047	\$64,508
Sulfuric Acid Storage Tank	12,600 gal, 12' dia x15' H		SS	1	\$96,000	2010	\$96,000	strm.A900.ACID-NET	1981	kg/hr	0.70	1.5	10,531	5.32	\$309,155	\$304,047	\$456,071
Caustic Storage Tank	12,600 gal, 12' dia x15' H		SS	1	\$96,000	2011	\$96,000	strm.A900.BASE-NET	1981	kg/hr	0.70	1.5	8,235	4.16	\$260,261	\$240,709	\$361,064
Firewater Storage Tank	600,000 gal - 4 hrs @ 2500 gpm		Glass lined	1	\$803,000	2009	\$803,000	strm.A900.H2O-FIRE	8343	kg/hr	0.70	1.7	8,343	1.00	\$803,000	\$833,464	\$1,416,890
Firewater Pump	2500 GPM, 150 FT TDH	125.0	CS	1	\$15,000	2009	\$15,000	strm.A900.H2O-FIRE	8343	kg/hr	0.80	3.1	8,343	1.00	\$15,000	\$15,569	\$48,264
Diesel storage tank	750,000 gal, 7 day storage, Floating roof		A285C	1	\$670,000	2009	\$670,000	strm.PR0-500	11341	kg/hr	0.70	1.7	11,465	1.01	\$675,160	\$700,774	\$1,191,317
Co-Product Storage Tank(Adipic)				1	\$690,900	2007	\$690,900	strm.PR0-700	23322.9025	kg/hr	0.65	1.850	10,798	0.46	\$418,819	\$431,812	\$798,852
Co-Product Storage Tank (Sodium Sulfate)				1	\$690,900	2007	\$690,900	strm.PR0-600	23322.9025	kg/hr	0.65	1.850	13,871	0.59	\$492,870	\$508,161	\$940,097
Glucose Storage Tank	70,000 gal		Glass lined	1	\$70,000	2009	\$70,000	strm.a400.401	1393	kg/hr	0.70	2.6	1,557	1.12	\$75,686	\$78,557	\$204,249
Area 900 Totals															\$9,861,551	\$9,894,800	\$17,195,641

BDO Pathway

A200: Pretreatment		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Flash Tank Agitator	Side-mounted, 3 x 75 hp. (170 kW)	170 kW	316LSS	3	\$90,000	2009	\$90,000	strm.a200.254	252891	kg/hr	0.50	1.5	192,146	0.76	\$78,450	\$81,426	\$122,139
Ammonia Addition Tank Agitator		10 hp	SS	1	\$21,900	2009	\$21,900	strm.a200.228	410369	kg/hr	0.50	1.5	230,647	0.56	\$16,418	\$17,041	\$25,562
Ammonia Static Mixer			SS	1	\$5,000	2009	\$5,000	strm.a200.275	157478	kg/hr	0.50	1.0	38,500	0.2445	\$2,472	\$2,566	\$2,566
Pretreatment Water Heater	29.9 MMBtu		304SS	1	\$92,000	2010	\$92,000	Heat.A200.QH201	-8	Gcal/hr	0.70	2.2	(0.29)	0.04	\$9,453	\$9,297	\$20,453
Pretreatment Sugar Beet extruder				1	\$5,424,000	2010	\$5,424,000	SCIS.a200.DEAC-IN	38600	kg/hr	1.00	1.0	70,483	1.83	\$9,904,187	\$9,740,555	\$9,740,555
Milling Equipment	200kg/dry ton			8	\$2,466,700	2013	\$2,466,700	SCIS.a200.211b	62942	kg/hr	0.60	1.5	57,306	0.91	\$19,733,600	\$18,843,101	\$28,264,651
Milling Equipment-Szego Mill				11	\$578,000	2013	\$578,000	SCIS.a200.211b	62942	kg/hr	0.60	1.4	57,306	0.91	\$6,358,000	\$6,071,089	\$8,499,524
Blowdown Tank Discharge Pump	1900 GPM, 150 FT TDH	125	316SS	1	\$25,635	2010	\$25,635	strm.a200.222	292407	kg/hr	0.80	2.3	193,144	0.66	\$18,397	\$18,093	\$41,614
Flash Tank Discharge Pump	900 GPM, 150 FT TDH	75	316SS	1	\$30,000	2009	\$30,000	strm.a200.254	204390	kg/hr	0.80	2.3	192,146	0.94	\$28,554	\$29,637	\$68,165
Deacetylation Tank Discharge Pump	1771 GPM, 150 FT TDH	100	316SS	1	\$22,500	2009	\$22,500	strm.a200.211a	402194	kg/hr	0.80	2.3	283,665	0.71	\$17,017	\$17,662	\$40,624
Hydrolyzate Pump	1771 GPM, 150 FT TDH	100	316SS	1	\$22,500	2009	\$22,500	strm.a200.228	402194	kg/hr	0.80	2.3	230,647	0.57	\$14,421	\$14,968	\$34,426
Deacetylation reactor conveyors	Feed and discharge drag conveyors	40 hp	SS316	3	\$110,000	2013	\$110,000	strm.a200.211a	277167	kg/hr	0.80	1.7	283,665	1.02	\$336,175	\$321,004	\$545,707
S/L Split Discharge Pump to WWT	900 GPM, 150 FT TDH	75	316SS	1	\$30,000	2009	\$30,000	strm.a200.4	204390	kg/hr	0.80	2.3	193,144	0.94	\$28,672	\$29,760	\$68,447
Flash Tank	23' x 48' - 110,000 gal.		SS316	1	\$511,000	2009	\$511,000	strm.a200.223	264116	kg/hr	0.70	2.0	193,144	0.73	\$410,470	\$426,042	\$852,084
Ammonia Addition Tank	118,000 gal., 1hr residence time		SS304	1	\$236,000	2009	\$236,000	strm.a200.228	410369	kg/hr	0.70	2.0	230,647	0.56	\$157,671	\$163,653	\$327,306
Area 200 Totals															\$37,113,956	\$35,785,895	\$48,653,825

A300: Hydrolysis and Fermentation		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Batch Enzymatic Hydrolysis																	
Hydrolyzate Cooler	Plate & Frame 32.5 MMBtu/hr		SS 304	1	\$85,000	2010	\$85,000	heat.A300.EH.GC301	8	Gcal/hr	0.70	2.2	6	0.78	\$71,116	\$69,941	\$153,871
Enzyme-Hydrolyzate Mixer	inline mixer 1673 gpm	100 hp	SS316	1	\$109,000	2009	\$109,000	strm.a300.EH.I310fd	379938	kg/hr	0.50	1.7	2	0.00	\$0	\$0	\$0
Saccharification Tank	250,000 gal each - 19' dia. x 120' tall		304SS	8	\$3,840,000	2009	\$3,840,000	strm.a300.EH.306	421776	kg/hr	0.70	2.0	238,222	0.56	2574312.593	\$2,671,978	\$5,343,955
Saccharification Transfer Pump	352 GPM, 150 FT TDH	20	316SS	5	\$47,200	2009	\$47,200	strm.a300.EH.306	421776	kg/hr	0.80	2.3	238,222	0.56	\$29,886	\$31,019	\$71,345
Lignin Filter (after enzymatic hydrolysis)	(4) 170 m2 Horizontal Belt Filters	660 hp ea	304SS	0	\$2,152,500	2013	\$0	scis.A300.EH.solid5	328984	kg/hr	1.00	1.7	1	1.00	\$0	\$0	\$0
Enzymatic Hydrolysis Storage Tank	1,200,000 gallon		316SS	1	\$1,317,325	2011	\$1,317,325	strm.a300.EH.306A	328984	kg/hr	0.70	1.8	238,222	0.72	\$1,050,891	\$971,944	\$1,749,500
Hydrolyzate Storage Transfer Pump	2152 GPM, 171 FT TDH	125 hp	316SS	1	\$26,800	2009	\$26,800	strm.a300.PROD-EH	488719	kg/hr	0.80	2.3	0	0.00	\$0	\$0	\$0
Filtered Hydrolyzate Storage Tank	300 hp		SS	1	\$51,600	2011	\$51,600	strm.a300.PROD-EH	348690	kg/hr	0.70	1.8	0	0.00	\$0	\$0	\$0
Fermenter Tank (saccharification contribution)			304SS	12	\$10,128,000	2009	\$10,128,000	NVESBDO	12	ea	1	1.50	6	0.476	\$4,817,202	\$4,999,959	\$7,499,938
Fermenter Agitator (saccharification contribution)		30 hp	SS304	1	\$52,500	2009	\$52,500	NVESBDO	1	ea	1	1.50	6	5.708	\$299,648	\$311,016	\$466,525
Fermentation Cooler (saccharification contrib)	Plate & frame		304SS	12	\$86,928	2009	\$86,928	NVESBDO	12	ea	1	2.20	6	0.476	\$41,346	\$42,914	\$94,412
Fermentation Recirc/Transfer Pump (saccharif)	340 GPM, 150 FT	20	316SS	5	\$47,200	2009	\$47,200	NVESBDO	12	ea	0.8	2.30	6	0.476	\$26,047	\$27,035	\$62,181
Area 300 Totals															\$8,910,449	\$9,125,808	\$15,441,726

A400: Enzyme Production		Mechanical Equipment List						Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Cellulase Fermenter Agitators		800.0	SS316		\$380,000	2009	\$380,000	CLVESSEL	1	ea	1.00	1.5	5	5.00	\$2,900,000	\$3,010,021	\$4,515,032
Cellulase Fermenter Agitators		0.75hp	SS316		\$3,420	2009	\$3,420	CLSEED	1	ea	1.00	1.5	4	4.00	\$13,680	\$14,298	\$21,298
Cellulase Fermenter Agitators		8 hp	SS316		\$11,000	2009	\$11,000	CLSEED	1	ea	1.00	1.5	4	4.00	\$44,000	\$45,669	\$68,504
Cellulase Fermenter Agitators		80 hp	SS316		\$63,000	2009	\$63,000	CLSEED	1	ea	1.00	1.5	4	4.00	\$252,000	\$261,560	\$392,341
Media-Prep Tank Agitator		7.5 hp	A285C	1	\$8,500	2009	\$8,500	strm.a400.402a	12255	kg/hr	0.50	1.5	0	0.00	\$0	\$0	\$0
Cellulase Nutrient Mix Tank Agitator		3 hp	CS	1	\$4,800	2009	\$4,800	strm.a400.416	174	kg/hr	0.50	1.6	123	0.70	\$4,030	\$4,182	\$6,692
Cellulase Hold Tank Agitator		10 hp	SS316	1	\$26,900	2009	\$26,900	strm.422	10930	kg/hr	0.50	1.5	7.575	0.69	\$23,395	\$23,244	\$34,866
Cellulase Fermentor	80,000 gal, 1 atm, 28 °C, Internal coil		SS316		\$400,500	2009	\$400,500	CLVESSEL	1	ea	1.00	2.0	5	5.00	\$2,002,500	\$2,078,471	\$4,156,943
1st Cellulase Seed Fermentor	80 gallon skid complete - \$46,000 ea		304SS		\$46,000	2009	\$46,000	CLSEED	1	ea	1.00	1.8	4	4.00	\$184,000	\$190,981	\$343,765
2nd Cellulase Seed Fermentor	800 gallon skid complete - \$57,500 ea		304SS		\$57,500	2009	\$57,500	CLSEED	1	ea	1.00	1.8	4	4.00	\$230,000	\$238,726	\$429,706
3rd Cellulase Seed Fermentor	8,000 gallon skid complete - \$95,400 ea		304SS		\$95,400	2009	\$95,400	CLSEED	1	ea	1.00	1.8	4	4.00	\$381,600	\$396,077	\$712,939
Cellulase Fermentation Cooler	Cooling coil included with Cellulase Fermentor		304SS		INCLUDED												
Media Prep Tank Cooler	Cooling coil included with Media Prep Tank		304SS	1	INCLUDED												
Fermenter Air Compressor Package	8000 SCFM @ 16 psig		CS	2	\$350,000	2009	\$350,000	strm.a400.450	33168	kg/hr	0.60	1.6	17.839	0.54	\$241,242	\$250,395	\$400,632
Cellulase Transfer Pump	59 gpm, 100 FT, TDH SIZE 2X1-10C	3	316SS	1	\$7,357	2010	\$7,357	strm.a400.422	13399	kg/hr	0.80	2.3	7.575	0.57	\$4,662	\$4,585	\$10,545
Cellulase Seed Pump	3 GPM, 100 FT TDH SIZE 2X1-10	2	316SS	4	\$29,972	2010	\$29,972	strm.a400.409	681	kg/hr	0.80	2.3	421	0.62	\$20,408	\$20,071	\$46,163
Cellulase Nutrient Transfer Pump	Gear Pump 2 GPM, 100 FT	1	316SS	1	\$1,500	2009	\$1,500	strm.a400.416	454	kg/hr	0.80	2.3	123	0.27	\$526	\$546	\$1,257
Cellulase Feed Pump	Gear Pump	1	316SS	1	\$5,700	2009	\$5,700	strm.a400.422	18168	kg/hr	0.80	2.3	7.575	0.42	\$2,831	\$2,938	\$6,759
Anti-foam Pump	Gear Pump 2 GPM, 100 FT	1	316SS	1	\$1,500	2009	\$1,500	strm.a400.444	11	kg/hr	0.80	2.3	7	0.69	\$1,115	\$1,157	\$2,661
Cellulase Nutrient Mix Tank	HDPE, 8,000 gal		HDPE	1	\$9,000	2010	\$9,000	strm.a400.416	224	kg/hr	0.70	3.0	123	0.55	\$5,806	\$5,806	\$17,417
Cellulase Hold Tank	80,000 gal		304SS	1	\$248,070	2009	\$248,070	strm.a400.422	10930	kg/hr	0.70	1.8	7.575	0.69	\$191,921	\$199,202	\$358,564
Area 400 Totals															\$6,502,813	\$6,747,832	\$11,526,084

A500: Bioconversion & Upgrading		Mechanical Equipment List										Scaled Installed Costs									
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Intr Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year				
BDO: Fermentation																					
Fermenter Feed Cooler	Plate & frame		SS304	1	\$86,928	2009	\$86,928	heat.A500.BDO-1.FERM.QC310	5.404	Gcal/hr	0.7	1.80	3	0.643	\$63,828	\$66,250	\$119,249				
Seed Hold Tank Agitator		15 hp	SS304	1	\$31,800	2009	\$31,800	strm.A500.BDO-1.FERM.304	40414	kg/hr	0.5	1.50	23,936	0.592	\$24,473	\$25,401	\$38,102				
4th Seed Vessel Agitator		7.5 hp	SS	2	\$26,000	2009	\$26,000	NSDBDO	2	ea	0.5	1.50	2	1.000	\$26,000	\$40,486	\$40,486				
5th Seed Vessel Agitator		10 hp	SS	2	\$43,000	2009	\$43,000	NSDBDO	2	ea	0.5	1.50	2	1.000	\$43,000	\$44,637	\$66,947				
Beer Surge Tank Agitator		20 hp	SS304	2	\$68,300	2009	\$68,300	strm.A500.BDO-1.FERM.PRD	425878	kg/hr	0.5	1.50	193,111	0.453	\$45,992	\$47,737	\$71,609				
1st Seed Fermentor	20 gallon skid complete - \$37,700 ea		304SS	2	\$75,400	2009	\$75,400	NSDBDO	2	ea	0.7	1.80	2	1.000	\$75,400	\$78,261	\$140,869				
2nd Seed Fermentor	200 gallon skid complete - \$58,300 ea		304SS	2	\$116,600	2009	\$116,600	NSDBDO	2	ea	0.7	1.80	2	1.000	\$116,600	\$121,024	\$217,842				
3rd Seed Fermentor	2000 gallon skid complete - \$78,800 ea		304SS	2	\$157,600	2009	\$157,600	NSDBDO	2	ea	0.7	1.80	2	1.000	\$157,600	\$163,579	\$294,442				
4th Seed Fermentor	20,000 gallon, incl. coil - \$176,000 ea		304SS	2	\$352,000	2009	\$352,000	NSDBDO	2	ea	0.7	2.00	2	1.000	\$352,000	\$363,579	\$730,709				
4th Seed Fermentor Coil	incl. w/ tank		304SS	1	INCLUDED			NSDBDO													
5th Seed Fermentor	200,000 gallon, incl. coil - \$590,000 ea		304SS	2	\$1,180,000	2009	\$1,180,000	NSDBDO	2	ea	0.7	2.00	2	1.000	\$1,180,000	\$1,224,767	\$2,449,534				
5th Seed Fermentor Coil	incl. w/ tank		304SS	1	INCLUDED																
Seed Hold Transfer Pump	190 GPM, 150 FT TDH	10	316SS	1	\$8,200	2009	\$8,200	strm.A500.BDO-1.FERM.304	43149	kg/hr	0.8	2.30	23,936	0.555	\$5,118	\$5,312	\$12,217				
Seed Hold Tank	300,000 gallon		316SS	1	\$439,000	2009	\$439,000	strm.A500.BDO-1.FERM.304	40414	kg/hr	0.7	1.80	23,936	0.592	\$304,248	\$315,791	\$568,424				
Seed Transfer Pump	190 GPM, 615 FT TDH	40	316SS	2	\$24,300	2009	\$24,300	strm.A500.BDO-1.FERM.304	43149	kg/hr	0.8	2.30	23,936	0.555	\$15,166	\$15,741	\$36,205				
Bioreactor Seed Blowers	750 SCFM @ 11psig	61 hp	CS	1	\$19,000	2013	\$19,000	NSDBDO	1	ea	0.6	1.60	3	2.000	\$28,799	\$27,499	\$43,998				
Fermentation Air Compr	scaled by ACFH, installed		CS	1	\$986,437	2013	\$0														
Fermenter Tank (Anaerobic)			304SS	12	\$10,128,000	2009	\$10,128,000	NVESBDO	12	ea	1	1.50	2	0.178	\$1,806,451	\$1,874,985	\$2,812,477				
Fermenter Agitator		30 hp	SS304	1	\$52,500	2009	\$52,500	NVESBDO	1	ea	1	1.50	2	0.178	\$112,368	\$116,631	\$174,947				
Fermentation Cooler	Plate & frame		304SS	12	\$86,928	2009	\$86,928	NVESBDO	12	ea	1	2.20	2	0.178	\$15,505	\$16,093	\$35,404				
Fermentation Recirc/Transfer Pump	340 GPM, 150 FT	20	316SS	5	\$47,200	2009	\$47,200	NVESBDO	12	ea	0.8	2.30	2	0.178	\$11,885	\$12,335	\$28,372				
Bioreactor Transfer Pump	2152 GPM, 171 FT TDH	125	316SS	1	\$26,800	2009	\$26,800	strm.A500.BDO-1.FERM.PRD	488719	kg/hr	0.8	2.30	193,111	0.395	\$12,751	\$13,234	\$30,439				
Bioreactor Storage Tank	1,200,000 gallon		316SS	1	\$1,317,325	2011	\$1,317,325	strm.A500.BDO-1.FERM.PRD	156789	kg/hr	0.7	1.80	193,111	1.232	\$1,524,184	\$1,409,681	\$2,537,426				
PSA				1	\$975,000	2013	\$975,000	strm.A500.BDO-1.FERM.FERM.VNT	13528	kg/hr	0.6	1.90	20,817	1.539	\$1,262,760	\$1,205,777	\$2,290,973				
BDO-SLS (whole slurry)																					
Filtrate Tank Agitator		7.5 hp	SS	1	\$26,000	2009	\$26,000	strm.A500.BDO-1.FERM.SLS.572	337439	kg/hr	0.5	1.5	193,111	0.5723	\$19,669	\$20,415	\$30,623				
Uginin Wet Cake Conveyor	Belt 100 ft. long x 24" wide, enclosed	10	SS304	1	\$70,000	2009	\$70,000	strm.A500.BDO-1.FERM.SLS.571	28630	kg/hr	0.80	1.7	24,927	0.8707	\$62,658	\$65,035	\$110,560				
Uginin Wet Cake Screw	Screw conveyor - 25 ft lg x 14" dia	15	SS304	1	\$20,000	2009	\$20,000	strm.A500.BDO-1.FERM.SLS.571	28630	kg/hr	0.80	1.7	24,927	0.8707	\$17,902	\$18,581	\$31,589				
Pressure Filter Pressing Compr	460 SCFM, 300 psig	150 hp	SS	1	\$75,000	2009	\$75,000	strm.A500.BDO-1.FERM.SLS.SQAINRIN	808	kg/hr	0.6	1.6	451	0.5776	\$52,968	\$54,977	\$87,964				
Pressure Filter Drying Compr	4000 SCFM, 130 psig (ea)	700 hp ea.	SS	2	\$405,000	2009	\$405,000	strm.A500.BDO-1.FERM.SLS.557	12233	kg/hr	0.60	1.6	6,743	0.5512	\$283,302	\$294,050	\$470,470				
Filtrate Tank Discharge Pump	590 GPM, 100 FT TDH SIZE 4X3-13		SS	1	\$13,040	2010	\$13,040	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.80	2.3	24,927	0.7835	\$10,728	\$10,551	\$24,266				
Feed Pump	1014 GPM 230 FT TDH SIZE 8X6-15	100 hp	SS	1	\$18,173	2010	\$18,173	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.80	2.3	24,927	0.7835	\$14,951	\$14,704	\$33,818				
Manifold Flush Pump		100 hp	SS	1	\$17,057	2010	\$17,057	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.80	2.3	24,927	0.7835	\$14,032	\$13,801	\$31,741				
Cloth Wash Pump		150 hp	SS	1	\$29,154	2010	\$29,154	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.80	2.3	24,927	0.7835	\$23,984	\$23,588	\$54,253				
Filtrate Discharge Pump	590 GPM, 100 FT TDH SIZE 4X3-13	75 hp	SS	1	\$13,040	2010	\$13,040	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.80	2.3	24,927	0.7835	\$10,728	\$10,551	\$24,266				
Pressure Filter	384 sq. m filtration area ea incl packing		SS316	2	\$3,294,700	2010	\$3,294,700	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.60	1.7	24,927	0.7835	\$2,710,482	\$2,665,701	\$4,531,692				
Filtrate Tank	13,750 gal 14' dia x 12' H		SS	1	\$103,000	2010	\$103,000	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.70	2.0	24,927	0.7835	\$86,829	\$85,394	\$170,789				
Feed Tank	20,300 gal 14' dia x 18' H		SS	1	\$174,800	2010	\$174,800	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.70	2.0	24,927	0.7835	\$147,356	\$144,922	\$289,843				
Recycled Water Tank	4000 gal.		HDPE	1	\$1,520	2010	\$1,520	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.70	3.0	24,927	0.7835	\$1,281	\$1,260	\$3,781				
Pressing Air Compressor Receiver	1350 gal., 300 psig design		CS	1	\$8,000	2010	\$8,000	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.70	3.1	24,927	0.7835	\$6,744	\$6,633	\$20,561				
Drying Air Compressor Receiver	9,000 gal., 150 psig design		CS	2	\$17,000	2010	\$17,000	strm.A500.BDO-1.FERM.SLS.571	31815	kg/hr	0.70	3.1	24,927	0.7835	\$14,331	\$14,094	\$43,692				
BDO-Dehydration and Oligomerization																					
Polishing Filter	Ceramic microfiltration		316L	4	\$440,000	2014	\$440,000	non water flow	53204	kg/hr	0.90	1.800	24,177	0.45	\$865,405	\$813,730	\$1,464,714				
liquid flow								strm.A500.BDO-1.FD-AQ													
water flow								cmix.H2O.A500.BDO-1.FD-AQ													
Polished Hydrolysate Storage Tank	8500 gal - 20 min residence time		SS	1	\$168,000	2011	\$168,000	non water flow	76712	kg/hr	0.70	1.800	24,177	0.32	\$74,866	\$69,241	\$124,635				
liquid flow								strm.A500.BDO-1.FD-AQ													
water flow								cmix.H2O.A500.BDO-1.FD-AQ													
Ion Exchange	Strong acid cation/weak base anion		SS	1	\$5,250,000	2014	\$5,250,000	non water flow	53204	kg/hr	0.90	1.800	24,177	0.45	\$2,581,464	\$2,427,320	\$4,369,175				
liquid flow								strm.A500.BDO-1.FD-AQ													
water flow								cmix.H2O.A500.BDO-1.FD-AQ													
Deionized Sugar Storage Tank	8500 gal - 20 min residence time		SS	1	\$168,000	2011	\$168,000	non water flow	76712	kg/hr	0.70	1.800	24,177	0.32	\$74,866	\$69,241	\$124,635				
liquid flow								strm.A500.BDO-1.FD-AQ													
water flow								cmix.H2O.A500.BDO-1.FD-AQ													
Aqueous upgrading Reactor	BC 2014 design report		317L Clad	1	\$2,044,000	2014	\$2,044,000	strm.A500.BDO-1.FD-AQ	53204	kg/hr	0.37	2.200	193,111	3.63	\$3,293,292	\$3,096,644	\$6,812,616				
HX BDO Feed-Btm Economizer	29.9 MMbtu		304SS	1	\$92,000	2010	\$92,000	heat.A500.BDO-1.AQUEOUS.24	7.8	Gcal/hr	0.70	2.200	216	2.00	\$149,368	\$146,300	\$323,181				
HX BDO Feed Trim Heater	9.4 MM btu/hr		304SS	1	\$92,000	2010	\$92,000	heat.A500.BDO-1.AQUEOUS.Q1-OG2	2.4	Gcal/hr	0.70	2.200	(32)	13.30	\$562,938	\$553,638	\$1,218,000				
Air Cooler (Fermenter Air Compressor Package)	8000 SCFM @ 16 psig		CS	2	\$350,000	2009	\$0	strm.A500.BDO-1.AQUEOUS.0G-21	33168	kg/hr	0.60	1.600	579	0.02	\$0	\$0	\$0				
H2 Makeup Compressor	reciprocating compressor(5 stages)	3162 hp	CS	1	\$2,900,000	2014	\$2,900,000	WORK.A500.BDO-1.AQUEOUS.11	2359	kW	0.87	1.90	1,524	0.65	\$2,003,918	\$1,884,260	\$3,880,200				
H2 Recycle Compressor	centrifugal compressor	6300 hp	CS	1	\$2,900,000	2014	\$2,900,000	WORK.A500.BDO-1.AQUEOUS.8	4700	kW	0.78	1.40	5,243	1.12	\$3,158,099	\$2,969,523	\$4,157,333				
KO Drum	(Based on ETJ report)		SS	1	\$72,474	2007	\$72,474	strm.A500.BDO-1.AQUEOUS.BUTENES	198788	kg/hr	0.65	3.630	193,772	0.97	\$71,280	\$73,491	\$266,774				
Distillation Column 23 BDO costed in IPE			304SS	1	\$1,387,516	2007	\$1,387,516	strm.A500.BDO-1.AQUEOUS.BUTENES	109821	kg/hr	0.60	1.138	193,772	1.76	\$1,950,751	\$2,021,271	\$2,287,966				
Reboiler	29.9 MMbtu		304SS	1	\$92,000	2010	\$92,000	heat.A500.BDO-1.HTREAT.Q-FURN	7.5	Gcal/hr	0.70	2.200	(13)	1.76	\$136,463	\$134,208	\$295,258				
Condenser	Plate & Frame 32.5 MMbtu/hr		SS 304	1	\$85,000	2010	\$85,000	strm.A500.BDO-1.AQUEOUS.Q1-OG2	8.2	Gcal/hr	0.70	2.200	49	5.93	\$293,451	\$289,651	\$639,451				
Air Cooler (Rectification Column Condenser)	8000 SCFM @ 16 psig		CS	1	\$487,000	2010	\$487,000	heat.A500.BDO-1.AQUEOUS.31	23	kg/hr	0.60	1.600	49	2.11	\$763,253	\$750,643	\$1,201,029				

A600: WWT		Mechanical Equipment List					Scaled Installed Costs										
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Aeration Basin	Concrete and steel, not installed cost		Concrete	3	\$4,804,854	2012	\$4,804,854	Hydraulic flow	2.7	MGD	0.60	2.1	2	0.81	\$4,236,252	\$3,925,381	\$8,125,539
Pump - Centrifugal, Aeration Basin Feed	852 gpm ea	45 hp	CS	4	\$64,800	2012											
Aeration Grid	Full floor aeration grid		CS	1	\$2,500,000	2012											
Cautic Feed System	15000 SCFM @ 10 Jaspie ea	1.5 hp	CS	4	\$20,000	2012	\$20,000	COD	5600	kg/hr	0.60	3.0	7.128	1.27	\$23,115	\$21,419	\$64,257
Blowers	Includes membrane, CIP, Scour system	1000 hp ea	CS	9	\$2,070,000	2012	\$2,070,000	COD	5600	kg/hr	0.60	2.0	7.128	1.27	\$2,892,448	\$2,216,881	\$4,433,763
Membrane Bioreactor		85 hp ea	CS	1	\$4,898,500	2012	\$4,898,500	Hydraulic flow	2.7	MGD	1.00	1.6	2	0.81	\$3,870,993	\$3,679,588	\$6,034,524
Pump, Centrifugal, MBR, RAS		160 hp	CS	6	INCLUDED	2012											
Gravity Belt Thickeners	2m presses	48hp	CS	3	\$750,000	2012	\$750,000	COD	5600	kg/hr	0.60	1.6	7.128	1.27	\$866,829	\$803,218	\$1,277,116
Centrifuge		165 hp ea	CS	1	\$686,800	2012	\$686,800	COD	5600	kg/hr	0.60	2.7	7.128	1.27	\$793,784	\$735,533	\$1,978,585
Pump, Centrifugal, Centrifuge Feed	105 gpm	15hp	CS	2	INCLUDED	2012											
Pump, Submersible, Centrate	100 gpm	10 hp ea	CS	2	INCLUDED	2012											
Dewatering Polymer Addition	9.8 gph neat polymer	1 hp ea	CS	2	INCLUDED	2012											
Conveyor		10 hp ea	CS	1	\$7,000	2012	\$7,000	COD	5600	kg/hr	0.60	2.9	7.128	1.27	\$8,090	\$7,497	\$21,441
Reverse Osmosis							\$2,450,000	Hydraulic flow	2.7	MGD	1.00	1.8	2	0.81	\$1,886,105	\$1,840,357	\$3,220,635
Evaporator	368 gpm	1480 hp ea	Titanium	1	\$5,000,000	2012	\$5,000,000	Hydraulic flow	2.7	MGD	0.60	1.6	2	0.81	\$4,408,905	\$4,084,808	\$6,576,541
Ammonia Addition System	0.63 gpm	4.5 hp	CS	4	\$195,200	2012	\$195,200	COD	5600	kg/hr	0.60	1.5	7.128	1.27	\$225,607	\$209,051	\$321,938
Sodium Sulfate Purification																	
Evaporator feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	strm.A600.23	290932	kg/hr	0.60	2.50	161,490	0.56	\$32,289	29862.98067	\$74,657
Evaporator feed heater	shell and tube 1/2 pass				\$274,818	2011	\$274,818	heat.A600.31	-13	MMkcal/	0.60	3.00	(5)	0.35	\$147,081	136031.67148	\$408,095
Evaporator flash drum	23 x 48' - 110,000 gal.		SS316	1	\$511,000	2009	\$511,000	strm.A600.23	264116	kg/hr	0.70	2.00	161,490	0.61	\$362,132	375870.7155	\$751,741
Centrifuge	Nexant quote sodium sulfate, 25410 lb/hr solids basis				\$327,680	2011	\$327,680	strm.A600.NA2504	11524	kg/hr	0.60	2.3	14,871	1.29	\$381,855	\$353,169	\$812,289
Dryer	Nexant quote Sodium sulfate, 25410 lb/hr solids basis				\$555,008	2011	\$555,008	strm.A600.PRD-SALT	11524	kg/hr	0.60	2.6	14,163	1.23	\$626,108	\$580,972	\$1,510,397
Area 600 Totals:															\$20,462,992	\$18,999,589	\$35,611,508

A700: Lignin Utilization		Mechanical Equipment List					Scaled Installed Costs										
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
A701: Lignin Conditioning																	
Neutralization Tank	2.6 atm, 130C operating @ 30 min. hold = 30,000 gal		SS317	1	\$236,000	2009	\$236,000	strm.A700.A701.LIQUID1	410369	kg/hr	0.70	2.0	83,860	0.20	\$77,657	\$80,603	\$161,206
Pulping Reactor Tank	2.6 atm, 130C operating (up to 160C, 30 min) @ 30 min. hold = 30,000 gal		SS316	1	\$16,300,000	2013	\$16,300,000	strm.A700.A701.PULP-OUT	323295	kg/hr	0.60	1.7	117,840	0.36	\$8,896,189	\$8,494,739	\$14,016,319
Flash/drain tank			SS317	1	\$262,000	2013	\$262,000	strm.A700.A701.PULP-OUT	323296	kg/hr	0.70	2.0	117,840	0.36	\$129,267	\$123,433	\$246,867
Black Liquor Storage Tank	1,200,000 gallon		316SS	1	\$1,317,325	2011	\$1,317,325	strm.A700.A701.5	328984	kg/hr	0.70	1.8	92,912	0.28	\$543,652	\$502,811	\$905,059
A702: Muconate Fermentation																	
1st Aerobic Seed	80 gallon skid complete - \$46,000 ea		304SS		\$46,000	2009	\$46,000	NSD1000	1	ea	1.00	1.80	3	3.00	\$130,260	\$143,225	\$257,824
1st Seed Vessel Agitator		0.75hp	SS316		\$3,420	2009	\$3,420	NSD1000	1	ea	1.00	1.50	3	3.00	\$10,649	\$10,649	\$15,974
2nd Aerobic Seed	800 gallon skid complete - \$57,500 ea		304SS		\$57,500	2009	\$57,500	NSD1000	1	ea	1.00	1.80	3	3.00	\$172,500	\$179,044	\$322,280
2nd Seed Vessel Agitator		8 hp	SS316		\$11,000	2009	\$11,000	NSD1000	1	ea	1.00	1.50	3	3.00	\$33,000	\$34,252	\$51,378
Bubble column seed fermenter	100 m3		316SS		\$274,100	2014	\$274,100	NSD1000	1	ea	1.00	2.30	3	3.00	\$822,300	\$773,199	\$1,778,358
Seed circulation cooler	650 sqft		316SS		\$8,400	2014	\$8,400	NSD1000	1	ea	1.00	2.20	3	3.00	\$25,200	\$23,695	\$52,130
Bubble column production fermenter	1000 m3		316SS		\$1,691,400	2014	\$1,691,400	NVES1000	1	ea	1.00	2.30	17	17.00	\$28,753,800	\$27,036,857	\$62,184,772
Production circulation cooler	4500 sqft		316SS		\$48,100	2014	\$48,100	NVES1000	1	ea	1.00	2.20	17	17.00	\$817,700	\$768,874	\$1,691,522
Production circulation pump	400 gpm		316SS		\$11,500	2014	\$11,500	NVES1000	1	ea	1.00	2.30	17	17.00	\$195,500	\$183,826	\$422,801
Fermentation air compressor	25,000 ACFM @ 45psig; max size in ACCE		CS		\$1,318,600	2014	\$1,318,600	ARV1000	13	m^3/s	1.00	1.60	15	1.14	\$1,503,850	\$1,414,052	\$2,262,484
Fermentation air receiver	25,000 gal		CS		\$104,600	2014	\$104,600	ARV1000	13	m^3/s	1.00	2.00	15	1.14	\$119,295	\$112,172	\$224,344
Fermentation Surge tank	insulated cone bottom, 6460 gal				\$45,966	2011	\$45,966	strm.A700.A702.UF-FD	290932	kg/hr	0.60	2.50	162,593	0.56	\$32,421	\$29,985	\$74,963
Ultrafiltration membrane separator					\$2,048,000	2011	\$2,048,000	Volume Flow	1303	GPM	0.60	2.50	701	1.00	\$2,048,000	\$1,894,146	\$4,735,366
membrane broth feed pump					INCLUDED			strm.A700.A702.UF-FD		kg/hr			162,593				
membrane solvent feed pump					INCLUDED			den.A700.A702.UF-FD		gm/cc			1				
A703: Recovery and Upgrading																	
Carbon Filter	2 Vessels, for color removal				\$345,234	2011	\$345,234	Volume Flow	1347	GPM	0.60	2.50	643	1.00	\$345,234	318298.7157	\$798,247
CCM Crystallizer	Olo Type, 2 in series		316SS	2 series	\$7,104,192	2011	\$7,104,192	Volume Flow	190	GPM	0.60	2.50	40	0.21	\$2,806,358	259523.628	\$6,488,824
CCM Centrifuge Separator					\$327,680	2011	\$327,680	strm.A700.A703.CRY1-PRD	13403	kg/hr	0.60	2.30	11,498	0.86	\$298,886	\$276,322	\$635,794
CCM Drier	Fluidized bed drier parallel			2	\$555,008	2011	\$555,008	strm.A700.A703.DRY1-PRD	11526	kg/hr	0.60	2.60	10,930	0.95	\$537,619	497231.3374	\$1,292,801
Dissolution Tank	mixing tank to redissolve crystals in solvent (EtOH)				\$1,317,325	2011	\$1,317,325	strm.A700.A703.FIL2-FD	328984	kg/hr	0.70	1.80	54,079	0.16	\$372,213	\$342,508	\$619,651
Dissolution Tank agitator	pump to retain crystal suspension	80	316SS		\$63,000	2009	\$63,000	work.A700.A703.W-ETOHMX	60	kW	1.00	1.50	60	1.00	\$63,000	65390.10165	\$98,085
Filtration Centrifuge(salt removal)	removes precipitated solids after dissolution				\$327,680	2011	\$327,680	strm.A700.A703.FIL2-SLT	13403	kg/hr	0.60	2.30	149	0.01	\$22,074	20415.25834	\$46,955
HDO feed tank	insulated, 6460 gal				\$45,966	2011	\$45,966	strm.A700.A703.FIL2-PRD	290932	kg/hr	0.60	2.50	53,930	0.19	\$16,721	15464.71724	\$38,662
HDO reactor pump					\$802,861	2014	\$802,861	strm.A700.A703.FIL2-PRD	208720	kg/hr	0.80	1.40	53,930	0.26	\$271,928	255889.0376	\$357,965
HDO Feed Effluent economizer	2-4 TEMA shell and tube HX		316SS		\$353,600	2011	\$353,600	heat.A700.A703.QH-HDO	14	MMkcal/	0.70	2.66	2	0.17	\$101,886	94232.11525	\$250,164
HDO trim preheater			304SS		\$41,000	2009	\$41,000	heat.A700.A703.QH-TRIM	-2	MMkcal/	0.70	2.20	-1	0.00	\$0	\$0	\$0
HDO Fixed Bed Reactor	(Q3 FY17 milestone), base PF=2.5,208 BBL/hr				\$4,168,568	2011	\$4,168,568	Volume Flow (liquid)	32895	L/hr	0.70	2.00	66,551	2.02	\$6,826,620	6313778.699	\$12,627,557
Pressure Factor (via Guthrie)	(>1000PSIG=2.5,900=2.3,800=1.9,700=1.8,600=1.6,500=1.45,400=1.35)			1.6	INCLUDED			strm.A700.A703.RXR-FD	29274	kg/hr			53,930				
Internals					INCLUDED			den.A700.A703.RXR-FD		1	G/M/CC		1				
Hydrogenation Intercooler (bed1)					\$2,353,181	2007	\$2,353,181	heat.A700.A703.QC-BED1	32	MMkcal/	0.65	2.21	2	0.05	\$356,676	367741.8853	\$812,710
Hydrogenation Intercooler (bed2)					\$2,353,181	2007	\$2,353,181	heat.A700.A703.QC-BED2	32	MMkcal/	0.65	2.21	3	0.09	\$484,357	499384.069	\$1,103,639
H2 Makeup Compressor	reciprocating compressor(5 stages)				\$1,621,200	2011	\$1,621,200	strm.A700.A703.H2-MU	390	kg/hr	0.60	1.09	406	1.04	\$1,061,679	1536846.949	\$1,674,966
H2 Makeup Compressor spare	reciprocating compressor(5 stages)				\$1,621,200	2011	\$1,621,200	heat.A700.A703.H2-MU	390	kg/hr	0.60	1.08	406	1.04	\$1,061,679	1536846.949	\$1,674,966
HHPS	Via Adipic model(via MB)				\$436,000	2013	\$436,000	strm.A700.A703.HHPS-FD	11984	kg/hr	1.00	1.50	54,338	0.45	\$197,681	188760.8762	\$283,141
HDO hot gas cooler					\$321,600	2011	\$321,600	heat.A700.A703.QAC-2	4	MMkcal/	0.70	1.66	-0	0.01	\$19,980	10155.55587	\$16,828
CHPS	3-Phase horizontal sep., demister, 3/16 SS316 cladding																

A800: CHP		Mechanical Equipment List					Scaled Installed Costs										
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
High Solids Burner and Turbine																	
Burner Combustion Air Preheater	INCLUDED			1	INCLUDED												
BFW Preheater	INCLUDED			1	INCLUDED												
Pretreatment/BFW heat recovery	9.4 MM Btu/hr		SS304	1	\$41,000	2009	\$41,000	heat.A800.A810.QH812	-2	Gcal/hr	0.70	2.2	(2)	0.66	\$30,504	\$31,662	\$69,655
Air Intake Fan	INCLUDED			1	INCLUDED												
Boiler	525,000 lb/hr @ 900 psig		CS	1	\$28,550,000	2010	\$28,550,000	strm.A800.A810.813c	238203	kg/hr	0.60	1.8	177,386	0.74	\$23,921,550	\$23,526,332	\$42,347,398
Combustion Gas Baghouse	Baghouse, Spray dryer scrubber, flues/ducting			1	\$11,000,000	2013	\$0	strm.A800.A810.812	238203	kg/hr	0.60	1.8	113,682	0.48	\$0	\$0	\$0
Turbine/Generator	23.6 kW, 2 extractions			1	\$9,500,000	2010	\$9,500,000	work.A900.wtotal	-42200	kW	0.60	1.8	(11,796)	0.28	\$4,421,675	\$4,348,623	\$7,827,521
Hot Process Water Softener System				1	\$78,000	2010	\$78,000	strm.A800.A810.812	235803	kg/hr	0.60	1.8	113,682	0.48	\$50,348	\$49,516	\$89,128
Amine Addition Pkg				1	\$40,000	2010	\$40,000	strm.A800.A810.812	235803	kg/hr	0.00	1.8	113,682	0.48	\$40,000	\$39,339	\$70,810
Ammonia Addition Pkg				1	INCLUDED												
Phosphate Addition Pkg				1	INCLUDED												
Condensate Pump			SS316	2	INCLUDED												
Turbine Condensate Pump			SS304	2	INCLUDED												
Deaerator Feed Pump			SS304	2	INCLUDED												
BFW Pump			SS316	5	INCLUDED												
Blowdown Pump			CS	2	INCLUDED												
Amine Transfer Pump			CS	1	INCLUDED												
Condensate Collection Tank			A285C	1	INCLUDED												
Condensate Surge Drum			SS304	1	INCLUDED												
Deaerator	Tray type		CS/SS316	1	\$305,000	2010	\$305,000	strm.A800.A810.812	235803	kg/hr	0.60	3.0	113,682	0.48	\$196,872	\$193,620	\$580,859
Blowdown Flash Drum			CS	1	INCLUDED												
Amine Drum			SS316	1	INCLUDED												
Area 800 Totals															\$28,660,950	\$28,189,091	\$50,985,372
A900: Utilities & Storage		Mechanical Equipment List					Scaled Installed Costs										
EQUIPMENT TITLE	DESCRIPTION	HP	MATERIAL	NUM REQD	\$	Year of Quote	Purch Cost in Base Yr	Scaling Variable	Scaling Val	Units	Scaling Exp	Inst Factor	New Val	Size Ratio	Scaled Purch Cost	Purch Cost in Proj year	Inst Cost in Proj year
Utilities System																	
Cooling Tower System	44,200 gpm	750 hp	FIBERGLASS	1	\$1,375,000	2010	\$1,375,000	strm.a900.945	10037820	kg/hr	0.60	1.5	10,448,831	1.04	\$1,408,509	\$1,385,239	\$2,077,858
Plant Air Compressor	400 SCFM@125 psig	150 hp		1	\$28,000	2010	\$28,000	DRY101	83333	kg/hr	0.60	1.6	83,333	1.00	\$28,000	\$27,537	\$44,060
Chilled Water Package	2 x 2350 tons (14.2 MM kcal/hr)	3400 hp		1	\$1,275,750	2010	\$1,275,750	heat.a900.qchwop	14	Gcal/hr	0.60	1.6	51	3.60	\$2,749,513	\$2,704,087	\$4,326,539
CIP System	100,000 GAL		SS304/SS31	1	\$423,000	2009	\$423,000	strm.a900.914	63	kg/hr	0.60	1.8	145	2.30	\$694,222	\$720,560	\$1,297,008
Cooling Water Pump	15,120 GPM, 100 FT TDH SIZE 20X20-28	500.0	CS	3	\$283,671	2010	\$283,671	strm.a900.945	10982556	kg/hr	0.80	3.1	10,448,831	0.95	\$272,588	\$268,084	\$831,061
Make-up Water Pump	685 GPM, 75 FT TDH SIZE 6X4-13	20.0	CS	1	\$6,864	2010	\$6,864	strm.a900.904	155564	kg/hr	0.80	3.1	445,086	2.86	\$15,945	\$15,652	\$48,521
Process Water Circulating Pump	2285 GPM, 75 FT TDH SIZE 6X6-13	75.0	CS	1	\$15,292	2010	\$15,292	strm.a900.905	538924	kg/hr	0.80	3.1	445,086	0.86	\$13,525	\$13,202	\$41,235
Instrument Air Dryer	670 SCFM - CYCLING TYPE		CS	1	\$15,000	2009	\$15,000	DRY101	83333	kg/hr	0.60	1.8	83,333	1.00	\$15,000	\$15,569	\$28,024
Plant Air Receiver	3800 gal - 72" x 228" vertical		CS	1	\$16,000	2009	\$16,000	DRY101	83333	kg/hr	0.60	3.1	83,333	1.00	\$16,000	\$16,607	\$51,482
Process Water Tank No. 1	250,000 gal		CS	1	\$250,000	2009	\$250,000	strm.a900.905	451555	kg/hr	0.70	1.7	445,086	0.99	\$247,488	\$256,877	\$436,691
Storage																	
Ammonia Storage Tank	28,000 gal		SA-516-70	2	\$196,000	2010	\$196,000	strm.A900.NH3-NET	1171	kg/hr	0.70	2.0	1,203	1.03	\$199,697	\$196,398	\$392,795
CSL Storage Tank	70,000 gal		Glass lined	1	\$70,000	2009	\$70,000	strm.A900.CSL-NET	1393	kg/hr	0.70	2.6	800	0.57	\$47,483	\$49,284	\$128,140
CSL Storage Tank Agitator		10 hp	SS304	1	\$21,200	2009	\$21,200	strm.A900.CSL-NET	1393	kg/hr	0.50	1.5	800	0.57	\$16,067	\$16,677	\$25,015
CSL Pump	8 GPM, 80 FT TDH	0.5	CS	1	\$3,000	2009	\$3,000	strm.A900.CSL-NET	1393	kg/hr	0.80	3.1	800	0.57	\$1,925	\$1,998	\$6,195
DAP Bulk Bag Unloader	Super sack unloader			1	\$30,000	2009	\$30,000	strm.A900.DAP-NET	163	kg/hr	0.60	1.7	627	3.84	\$67,301	\$69,854	\$118,753
DAP Bulk Bag Holder	Super sack holder			1	INCLUDED												
DAP Make-up Tank	12,800 gal		SS304	1	\$102,000	2009	\$102,000	strm.A900.DAP-NET	1615	kg/hr	0.70	1.8	627	0.39	\$52,577	\$54,572	\$98,229
DAP Make-up Tank Agitator		5.5 hp	SS304	1	\$9,800	2009	\$9,800	strm.A900.DAP-NET	163	kg/hr	0.50	1.5	627	3.84	\$19,215	\$19,944	\$29,916
DAP Pump	2 GPM, 100 FT TDH	0.5	CS	1	\$3,000	2009	\$3,000	strm.A900.DAP-NET	163	kg/hr	0.80	3.1	627	3.84	\$8,810	\$9,145	\$28,348
Sulfuric Acid Pump	5 GPM, 150 FT TDH SIZE 2X1-10	0.5	SS316	1	\$7,493	2010	\$7,493	strm.A900.ACID-NET	1981	kg/hr	0.80	2.3	10,835	5.47	\$29,175	\$28,693	\$65,993
Sulfuric Acid Storage Tank	12,600 gal, 12' dia x15' H		SS	1	\$96,000	2010	\$96,000	strm.A900.ACID-NET	1981	kg/hr	0.70	1.5	10,835	5.47	\$315,376	\$310,165	\$465,248
Caustic Storage Tank	12,600 gal, 12' dia x15' H		SS	1	\$96,000	2011	\$96,000	strm.A900.BASE-NET	1981	kg/hr	0.70	1.5	8,494	4.29	\$265,969	\$245,988	\$368,982
Firewater Storage Tank	600,000 gal - 4 hrs @ 2500 gpm		Glass lined	1	\$803,000	2009	\$803,000	strm.A900.H2O-FIRE	8343	kg/hr	0.70	1.7	8,343	1.00	\$803,000	\$833,464	\$1,416,890
Firewater Pump	2500 GPM, 150 FT TDH	125.0	CS	1	\$15,000	2009	\$15,000	strm.A900.H2O-FIRE	8343	kg/hr	0.80	3.1	8,343	1.00	\$15,000	\$15,569	\$48,264
Diesel storage tank	750,000 gal., 7 day storage, Floating roof		A285C	1	\$670,000	2009	\$670,000	strm.PRD-500	11341	kg/hr	0.70	1.7	11,032	0.97	\$657,171	\$682,103	\$1,159,575
Co-Product Storage Tank(Adipic)				1	\$690,900	2007	\$690,900	strm.PRD-700	23322.90249	kg/hr	0.65	1.850	11,121	0.476832101	\$426,926	\$440,171	\$814,317
Co-Product Storage Tank (Sodium Sulfate)				1	\$690,900	2007	\$690,900	strm.PRD-600	23322.90249	kg/hr	0.65	1.850	14,163	0.607255778	\$499,582	\$515,081	\$952,900
Glucose Storage Tank	70,000 gal		Glass lined	1	\$70,000	2009	\$70,000	strm.a400.401	1393	kg/hr	0.70	2.6	1,557	1.12	\$75,686	\$78,557	\$204,249
Area 900 Totals															\$8,961,720	\$8,991,177	\$15,506,286

Appendix B. Discounted Cash Flow Rate of Return Worksheet

Acids Pathway

DCFROR Worksheet									
Year	-2	-1	0	1	2	3	4	5	
Fixed Capital Investment	\$23,058,129	\$172,935,966	\$92,232,515						
Land	\$1,848,000								
Working Capital			\$36,028,326						
Loan Payment				\$64,431,397	\$64,431,397	\$64,431,397	\$64,431,397	\$64,431,397	\$64,431,397
Loan Interest Payment	\$2,766,975	\$23,519,291	\$34,587,193	\$34,587,193	\$32,199,657	\$29,621,118	\$26,836,296	\$23,828,687	\$23,828,687
Loan Principal	\$34,587,193	\$293,991,143	\$432,339,916	\$402,495,713	\$370,263,973	\$335,453,694	\$297,858,593	\$257,255,884	\$257,255,884
Fuel Sales				\$60,641,497	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330
By-Product Credit				\$132,885,303	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404
Total Annual Sales				\$193,526,801	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734
Annual Manufacturing Cost									
Feedstock				\$38,712,485	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)				\$16,959,502	\$0	\$1,993,834	\$238,632	\$1,993,834	\$1,993,834
Other Variable Costs				\$76,292,843	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821
Fixed Operating Costs				\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111
Total Product Cost				\$151,937,942	\$158,781,579	\$160,775,413	\$159,020,211	\$160,775,413	\$160,775,413
Annual Depreciation									
General Plant Writedown				14%	24.49%	17.49%	12.49%	8.93%	
Depreciation Charge				\$96,006,764	\$164,535,036	\$117,505,830	\$83,913,540	\$59,995,830	\$59,995,830
Remaining Value				\$575,839,032	\$411,303,997	\$293,798,167	\$209,884,627	\$149,888,797	\$149,888,797
Steam Plant Writedown				3.75%	7.22%	6.68%	6.18%	5.71%	
Depreciation Charge				\$1,827,027	\$3,517,150	\$3,253,083	\$3,009,480	\$2,783,415	\$2,783,415
Remaining Value				\$46,893,703	\$43,376,553	\$40,123,470	\$37,113,991	\$34,330,575	\$34,330,575
Net Revenue				(\$90,832,126)	(\$100,997,687)	(\$53,119,710)	(\$14,743,792)	\$10,652,388	\$10,652,388
Losses Forward					(\$90,832,126)	(\$191,829,813)	(\$244,949,523)	(\$259,693,315)	(\$259,693,315)
Taxable Income				(\$90,832,126)	(\$191,829,813)	(\$244,949,523)	(\$259,693,315)	(\$249,040,927)	(\$249,040,927)
Income Tax				\$0	\$0	\$0	\$0	\$0	\$0
Annual Cash Income				-\$22,842,538	\$34,822,758	\$32,828,924	\$34,584,126	\$32,828,924	\$32,828,924
Discount Factor		1.2100	1.1000	1.0000	0.9091	0.8264	0.7513	0.6830	0.6209
Annual Present Value	\$410,262,637			-\$20,765,943	\$28,779,139	\$24,664,857	\$23,621,424	\$20,384,179	\$20,384,179
Total Capital Investment + Interest	\$33,484,456	\$216,100,784	\$162,848,035						
Net Present Worth				\$0					

DCFROR Worksheet									
Year	6	7	8	9	10	11	12	13	
Fixed Capital Investment									
Land									
Working Capital									
Loan Payment	\$64,431,397	\$64,431,397	\$64,431,397	\$64,431,397	\$64,431,397	\$0	\$0	\$0	\$0
Loan Interest Payment	\$20,580,471	\$17,072,397	\$13,283,677	\$9,191,859	\$4,772,696	\$0	\$0	\$0	\$0
Loan Principal	\$213,404,958	\$166,045,958	\$114,898,238	\$59,658,701	\$0	\$0	\$0	\$0	\$0
Fuel Sales	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330
By-Product Credit	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404
Total Annual Sales	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734
Annual Manufacturing Cost									
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$511,169	\$2,232,466	\$0	\$1,993,834	\$238,632	\$2,505,003	\$0	\$2,232,466	\$2,232,466
Other Variable Costs	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821
Fixed Operating Costs	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111
Total Product Cost	\$159,292,748	\$161,014,045	\$158,781,579	\$160,775,413	\$159,020,211	\$161,286,582	\$158,781,579	\$161,014,045	\$161,014,045
Annual Depreciation									
General Plant Writedown	8.92%	8.93%	4.46%						
Depreciation Charge	\$59,928,645	\$59,995,830	\$29,964,323						
Remaining Value	\$89,960,152	\$29,964,323	\$0						
Steam Plant Writedown	5.29%	4.89%	4.52%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%
Depreciation Charge	\$2,574,891	\$2,381,469	\$2,203,151	\$2,173,919	\$2,173,432	\$2,173,919	\$2,173,432	\$2,173,919	\$2,173,919
Remaining Value	\$31,755,685	\$29,374,215	\$27,171,064	\$24,997,145	\$22,823,713	\$20,649,794	\$18,476,363	\$16,302,444	\$16,302,444
Net Revenue	\$15,658,980	\$17,571,993	\$53,803,004	\$85,894,543	\$92,069,395	\$94,575,233	\$97,080,723	\$94,847,770	\$94,847,770
Losses Forward	(\$249,040,927)	(\$233,381,947)	(\$215,809,954)	(\$162,006,949)	-\$76,112,407	\$0	\$0	\$0	\$0
Taxable Income	(\$233,381,947)	(\$215,809,954)	(\$162,006,949)	-\$76,112,407	\$15,956,989	\$94,575,233	\$97,080,723	\$94,847,770	\$94,847,770
Income Tax	\$0	\$0	\$0	\$0	\$3,350,968	\$19,860,799	\$20,386,952	\$19,918,032	\$19,918,032
Annual Cash Income	\$34,311,590	\$32,590,292	\$34,822,758	\$32,828,924	\$31,233,159	\$76,888,353	\$78,867,203	\$77,103,657	\$77,103,657
Discount Factor	0.5645	0.5132	0.4665	0.4241	0.3855	0.3505	0.3186	0.2897	0.2897
Annual Present Value	\$19,367,998	\$16,723,973	\$16,245,074	\$13,922,669	\$12,041,735	\$26,948,899	\$25,129,521	\$22,334,183	\$22,334,183
Total Capital Investment + Interest									
Net Present Worth									

DCFROR Worksheet

Year	14	15	16	17	18	19	20	21
Fixed Capital Investment								
Land								
Working Capital								
Loan Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Interest Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Principal	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Fuel Sales	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330
By-Product Credit	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404
Total Annual Sales	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734
Annual Manufacturing Cost								
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$0	\$1,993,834	\$749,801	\$1,993,834	\$0	\$2,232,466	\$0	\$2,505,003
Other Variable Costs	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821
Fixed Operating Costs	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111
Total Product Cost	\$158,781,579	\$160,775,413	\$159,531,380	\$160,775,413	\$158,781,579	\$161,014,045	\$158,781,579	\$161,286,582
Annual Depreciation								
General Plant Writedown								
Depreciation Charge								
Remaining Value								
Steam Plant Writedown	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	2.23%
Depreciation Charge	\$2,173,432	\$2,173,919	\$2,173,432	\$2,173,919	\$2,173,432	\$2,173,919	\$2,173,432	\$1,086,959
Remaining Value	\$14,129,012	\$11,955,093	\$9,781,661	\$7,607,742	\$5,434,310	\$3,260,391	\$1,086,959	\$0
Net Revenue	\$97,080,723	\$95,086,402	\$96,330,923	\$95,086,402	\$97,080,723	\$94,847,770	\$97,080,723	\$95,662,193
Losses Forward	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Taxable Income	\$97,080,723	\$95,086,402	\$96,330,923	\$95,086,402	\$97,080,723	\$94,847,770	\$97,080,723	\$95,662,193
Income Tax	\$20,386,952	\$19,968,144	\$20,229,494	\$19,968,144	\$20,386,952	\$19,918,032	\$20,386,952	\$20,089,060
Annual Cash Income	\$78,867,203	\$77,292,176	\$78,274,861	\$77,292,176	\$78,867,203	\$77,103,657	\$78,867,203	\$76,660,092
Discount Factor	0.2633	0.2394	0.2176	0.1978	0.1799	0.1635	0.1486	0.1351
Annual Present Value	\$20,768,200	\$18,503,133	\$17,034,890	\$15,291,845	\$14,184,960	\$12,607,064	\$11,723,107	\$10,359,122
Total Capital Investment + Interest								
Net Present Worth								

DCFROR Worksheet

Year	22	23	24	25	26	27	28	29	30
Fixed Capital Investment									
Land									(\$1,848,000)
Working Capital									(\$36,028,326)
Loan Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Interest Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Principal	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Fuel Sales	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330	\$80,855,330
By-Product Credit	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404	\$177,180,404
Total Annual Sales	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734	\$258,035,734
Annual Manufacturing Cost									
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$238,632	\$1,993,834	\$0	\$2,232,466	\$511,169	\$1,993,834	\$238,632	\$1,993,834	\$0
Other Variable Costs	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821	\$87,191,821
Fixed Operating Costs	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111	\$19,973,111
Total Product Cost	\$159,020,211	\$160,775,413	\$158,781,579	\$161,014,045	\$159,292,748	\$160,775,413	\$159,020,211	\$160,775,413	\$158,781,579
Annual Depreciation									
General Plant Writedown									
Depreciation Charge									
Remaining Value									
Steam Plant Writedown									
Depreciation Charge									
Remaining Value									
Net Revenue	\$99,015,523	\$97,260,321	\$99,254,155	\$97,021,689	\$98,742,986	\$97,260,321	\$99,015,523	\$97,260,321	\$99,254,155
Losses Forward	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Taxable Income	\$99,015,523	\$97,260,321	\$99,254,155	\$97,021,689	\$98,742,986	\$97,260,321	\$99,015,523	\$97,260,321	\$99,254,155
Income Tax	\$20,793,260	\$20,424,667	\$20,843,373	\$20,374,555	\$20,736,027	\$20,424,667	\$20,793,260	\$20,424,667	\$20,843,373
Annual Cash Income	\$78,222,263	\$76,835,653	\$78,410,782	\$76,647,134	\$78,006,959	\$76,835,653	\$78,222,263	\$76,835,653	\$78,410,782
Discount Factor	0.1228	0.1117	0.1015	0.0923	0.0839	0.0763	0.0693	0.0630	0.0573
Annual Present Value	\$9,609,290	\$8,580,864	\$7,960,702	\$7,074,224	\$6,545,209	\$5,860,846	\$5,424,194	\$4,843,674	\$4,493,609
Total Capital Investment + Interest									(\$2,170,637)
Net Present Worth									

BDO Pathway

DCFRR Worksheet

Year	-2	-1	0	1	2	3	4	5
Fixed Capital Investment								
Land	\$21,178,631	\$158,839,736	\$84,714,526					
Working Capital			\$33,091,612					
Loan Payment				\$59,179,512	\$59,179,512	\$59,179,512	\$59,179,512	\$59,179,512
Loan Interest Payment	\$2,541,436	\$21,602,204	\$31,767,947	\$31,767,947	\$29,575,022	\$27,206,663	\$24,648,835	\$21,886,381
Loan Principal	\$31,767,947	\$270,027,551	\$397,099,340	\$369,687,775	\$340,083,286	\$308,110,437	\$273,579,760	\$236,286,630
Fuel Sales				\$57,986,495	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327
By-Product Credit				\$136,749,562	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749
Total Annual Sales				\$194,736,057	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077
Annual Manufacturing Cost								
Feedstock				\$38,712,485	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)				\$17,572,041	\$2,061,224	\$2,501,573	\$2,299,856	\$2,501,573
Other Variable Costs				\$84,345,655	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034
Fixed Operating Costs				\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716
Total Product Cost				\$159,321,897	\$168,764,621	\$169,003,253	\$169,003,253	\$169,204,970
Annual Depreciation								
General Plant Writedown				14%	24.49%	17.49%	12.49%	8.93%
Depreciation Charge				\$87,290,016	\$149,596,396	\$106,837,116	\$76,294,773	\$54,548,625
Remaining Value				\$523,556,844	\$373,960,448	\$267,123,332	\$190,828,559	\$136,279,935
Steam Plant Writedown				3.75%	7.22%	6.68%	6.18%	5.71%
Depreciation Charge				\$1,911,951	\$3,680,634	\$3,404,293	\$3,149,366	\$2,912,794
Remaining Value				\$49,073,421	\$45,392,787	\$41,988,493	\$38,839,127	\$35,926,333
Net Revenue				(\$85,555,755)	(\$91,968,596)	(\$47,004,966)	(\$13,448,150)	\$11,095,307
Losses Forward					(\$85,555,755)	(\$177,524,351)	(\$224,529,317)	(\$237,977,467)
Taxable Income				(\$85,555,755)	(\$177,524,351)	(\$224,529,317)	(\$237,977,467)	(\$226,882,160)
Income Tax				\$0	\$0	\$0	\$0	\$0
Annual Cash Income				-\$23,765,351	\$31,703,944	\$31,263,595	\$31,465,312	\$31,263,595
Discount Factor		1.2100	1.1000	1.0000	0.9091	0.8264	0.7513	0.6830
Annual Present Value	\$376,995,241			-\$21,604,865	\$26,201,607	\$23,488,802	\$21,491,232	\$19,412,233
Total Capital Investment + Interest	\$30,937,361	\$198,486,134	\$149,574,085					
Net Present Worth				\$0				

DCFRR Worksheet

Year	6	7	8	9	10	11	12	13
Fixed Capital Investment								
Land								
Working Capital								
Loan Payment	\$59,179,512	\$59,179,512	\$59,179,512	\$59,179,512	\$59,179,512	\$0	\$0	\$0
Loan Interest Payment	\$18,902,930	\$15,680,804	\$12,200,907	\$8,442,619	\$4,383,668	\$0	\$0	\$0
Loan Principal	\$196,010,049	\$152,511,341	\$105,532,737	\$54,795,844	\$0	\$0	\$0	\$0
Fuel Sales	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327
By-Product Credit	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749
Total Annual Sales	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077
Annual Manufacturing Cost								
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$2,572,392	\$2,740,205	\$2,061,224	\$2,501,573	\$2,299,856	\$3,012,742	\$2,061,224	\$2,740,205
Other Variable Costs	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034
Fixed Operating Costs	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716
Total Product Cost	\$169,275,789	\$169,443,602	\$168,764,621	\$169,204,970	\$169,003,253	\$169,716,139	\$168,764,621	\$169,443,602
Annual Depreciation								
General Plant Writedown	8.92%	8.93%	4.46%					
Depreciation Charge	\$54,487,540	\$54,548,625	\$27,243,770					
Remaining Value	\$81,792,395	\$27,243,770	\$0					
Steam Plant Writedown	5.29%	4.89%	4.52%	4.46%	4.46%	4.46%	4.46%	4.46%
Depreciation Charge	\$2,694,577	\$2,492,165	\$2,305,559	\$2,274,967	\$2,274,457	\$2,274,967	\$2,274,457	\$2,274,967
Remaining Value	\$33,231,756	\$30,739,591	\$28,434,032	\$26,159,065	\$23,884,607	\$21,609,640	\$19,335,183	\$17,060,215
Net Revenue	\$14,287,240	\$17,482,881	\$49,133,220	\$79,725,520	\$83,986,699	\$87,656,970	\$88,608,998	\$87,929,507
Losses Forward	(\$226,882,160)	(\$212,594,920)	(\$195,112,040)	(\$145,978,820)	-\$66,253,299	\$0	\$0	\$0
Taxable Income	(\$212,594,920)	(\$195,112,040)	(\$145,978,820)	-\$66,253,299	\$17,733,399	\$87,656,970	\$88,608,998	\$87,929,507
Income Tax	\$0	\$0	\$0	\$0	\$3,724,014	\$18,407,964	\$18,607,890	\$18,465,196
Annual Cash Income	\$31,192,776	\$31,024,963	\$31,703,944	\$31,263,595	\$27,741,298	\$71,523,974	\$72,275,566	\$71,739,278
Discount Factor	0.5645	0.5132	0.4665	0.4241	0.3855	0.3505	0.3186	0.2897
Annual Present Value	\$17,607,509	\$15,920,712	\$14,790,124	\$13,258,816	\$10,695,471	\$25,068,717	\$23,029,223	\$20,780,313
Total Capital Investment + Interest								
Net Present Worth								

DCFROR Worksheet

Year	14	15	16	17	18	19	20	21
Fixed Capital Investment								
Land								
Working Capital								
Loan Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Interest Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Principal	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Fuel Sales	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327
By-Product Credit	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749
Total Annual Sales	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077
Annual Manufacturing Cost								
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$2,061,224	\$2,501,573	\$2,811,024	\$2,501,573	\$2,061,224	\$2,740,205	\$2,061,224	\$3,012,742
Other Variable Costs	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034
Fixed Operating Costs	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716
Total Product Cost	\$168,764,621	\$169,204,970	\$169,514,421	\$169,204,970	\$168,764,621	\$169,443,602	\$168,764,621	\$169,716,139
Annual Depreciation								
General Plant Writedown								
Depreciation Charge								
Remaining Value								
Steam Plant Writedown	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	4.46%	2.23%
Depreciation Charge	\$2,274,457	\$2,274,967	\$2,274,457	\$2,274,967	\$2,274,457	\$2,274,967	\$2,274,457	\$1,137,484
Remaining Value	\$14,785,758	\$12,510,791	\$10,236,333	\$7,961,366	\$5,686,908	\$3,411,941	\$1,137,484	\$0
Net Revenue	\$88,608,998	\$88,168,139	\$87,859,198	\$88,168,139	\$88,608,998	\$87,929,507	\$88,608,998	\$88,794,454
Losses Forward	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Taxable Income	\$88,608,998	\$88,168,139	\$87,859,198	\$88,168,139	\$88,608,998	\$87,929,507	\$88,608,998	\$88,794,454
Income Tax	\$18,607,890	\$18,515,309	\$18,450,432	\$18,515,309	\$18,607,890	\$18,465,196	\$18,607,890	\$18,646,835
Annual Cash Income	\$72,275,566	\$71,927,797	\$71,683,224	\$71,927,797	\$72,275,566	\$71,739,278	\$72,275,566	\$71,285,102
Discount Factor	0.2633	0.2394	0.2176	0.1978	0.1799	0.1635	0.1486	0.1351
Annual Present Value	\$19,032,415	\$17,218,943	\$15,600,358	\$14,230,531	\$12,999,396	\$11,729,945	\$10,743,302	\$9,632,797
Total Capital Investment + Interest								
Net Present Worth								

DCFROR Worksheet

Year	22	23	24	25	26	27	28	29	30
Fixed Capital Investment									
Land									(\$1,848,000)
Working Capital									(\$33,091,612)
Loan Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Interest Payment	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Loan Principal	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Fuel Sales	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327	\$77,315,327
By-Product Credit	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749	\$182,332,749
Total Annual Sales	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077	\$259,648,077
Annual Manufacturing Cost									
Feedstock	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647	\$51,616,647
Periodic Costs (Catalyst, etc)	\$2,299,856	\$2,501,573	\$2,061,224	\$2,740,205	\$2,572,392	\$2,501,573	\$2,299,856	\$2,501,573	\$2,061,224
Other Variable Costs	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034	\$96,395,034
Fixed Operating Costs	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716	\$18,691,716
Total Product Cost	\$169,003,253	\$169,204,970	\$168,764,621	\$169,443,602	\$169,275,789	\$169,204,970	\$169,003,253	\$169,204,970	\$168,764,621
Annual Depreciation									
General Plant Writedown									
Depreciation Charge									
Remaining Value									
Steam Plant Writedown									
Depreciation Charge									
Remaining Value									
Net Revenue	\$90,644,824	\$90,443,106	\$90,883,456	\$90,204,474	\$90,372,287	\$90,443,106	\$90,644,824	\$90,443,106	\$90,883,456
Losses Forward	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0	\$0
Taxable Income	\$90,644,824	\$90,443,106	\$90,883,456	\$90,204,474	\$90,372,287	\$90,443,106	\$90,644,824	\$90,443,106	\$90,883,456
Income Tax	\$19,035,413	\$18,993,052	\$19,085,526	\$18,942,940	\$18,978,180	\$18,993,052	\$19,035,413	\$18,993,052	\$19,085,526
Annual Cash Income	\$71,609,411	\$71,450,054	\$71,797,930	\$71,261,535	\$71,394,107	\$71,450,054	\$71,609,411	\$71,450,054	\$71,797,930
Discount Factor	0.1228	0.1117	0.1015	0.0923	0.0839	0.0763	0.0693	0.0630	0.0573
Annual Present Value	\$8,796,928	\$7,979,410	\$7,289,328	\$6,577,154	\$5,990,355	\$5,450,045	\$4,965,636	\$4,504,169	\$4,114,636
Total Capital Investment + Interest									(\$2,002,339)
Net Present Worth									

Appendix C. Process Parameters/Operating Summary

Acids Pathway

Final Fuel Product	
Fuel Mass flow (kg/hr)	11465.5
Estimated Density (kg/L)	0.6
Fuel Volume Flow (L/hr)	18792.0
Fuel LHV (MmKcal/hr)	120.5
Annual Fuel Volume (MM Gal/yr)	39.1
Annual Fuel GGE (MM GGE/yr)	32.5

A100: Feedstock	
Moisture Content	20%
Composition (wt% Dry Feed)	
Cellulose	35.0%
Xylan	19.5%
Arabinan	2.4%
Sucrose	0.8%
Lignin	15.8%
Acetate	1.8%
Extract	14.6%
Ash	4.9%
Mannan	0.6%
Galactan	1.4%
Protein	3.1%
Hydrolysis Mass yield (g/g biopolymer)	
Cellulose to glucose	1.111109
Xylan to xylose	1.136361
Arabinan to arabinose	1.136361

A200: Deacetylation & Pretreatment	
Deacetylation Conditions	
Temperature (C)	90
Pressure (atm)	1
NaOH loading (mg/L)	70
Solubilization to the Black Liquor	
Acetate	100%
Lignin	47.0%
Cellulose	2.0%
Xylan	10.0%
Arabinan	30.0%

A300: Continuous Enzymatic Hydrolysis	
Operating Conditiond	
Enzyme Loading	9.96
Hydrolysis CEH	
Cellulose conversion	96.3%
Xylan conversion	98.8%
Arabinan conversion	98.8%
Lignin Press	
Sugar Recovery (% inlet)	95.3%
Conditioning	
Feed Sugar Titer (g/L)	54.8
Concentrated Sugar Titer (g/L)	705.6

A500: C4 Acids Fermentation	
Contamination Sugar Loss	3.0%
Utilization	
Glucose	100.0%
Xylose	100.0%
Arabinose	87.4%
Sucrose	100.0%
Diversion of substrate to Biomass (% of substrate Utilized)	
Glucose	5.0%
Xylose	15.0%
Arabinose	2.0%
Sucrose	5.0%
Diversion of substrate to Product (% of substrate Utilized)	
Glucose	95.0%
Xylose	85.0%
Arabinose	85.4%
Sucrose	95.0%
Maximum theoretical metabolic yield (g/g)	
Glucose to Butyric	0.489
Glucose to Biomass	0.820
Xylose to Butyric	0.489
Xylose to Biomass	0.820
Arabinose to Butyric	0.489
Arabinose to Biomass	0.820
Sucrose to Butyric	0.489
Sucrose to Biomass	0.863
Net Metabolic Yield (g/g substrate consumed)	
Glucose to Butyric	0.4646
Glucose to Biomass	0.0410
Xylose to Butyric	0.4156
Xylose to Biomass	0.1230
Arabinose to Butyric	0.4176
Arabinose to Biomass	0.0164
Sucrose to Butyric	0.4646
Sucrose to Biomass	0.0432
Extraction Metrics	
HFMC Organic loading (kg Org/kg Aq)	0.10
Butyric Acid Recovery (% feed)	1.00

A500: Acid Catalytic Upgrading	
Theoretical Yields , Fuel upgading	
Acid condensation (g ketone/g acid)	0.648
Ketone condensation (g enone/g ketone)	0.9211
Enone hydrogenation (g hydrocarbon/g enone)	0.943
Acid Condensation	
Temperature (C)	321.52
Pressure (atm)	1
Butyric to 4-Heptanone (kg/kg)	0.65
Ketone Condensation	
Temperature (C)	180
Pressure (atm)	11.21
Toluene:Ketone Ratio	3.63
4-Heptanone to C13-Enone (kg/kg)	0.92
Enone Hydrogenation	
Temperature (C)	270.00
Pressure (atm)	35.70
H2:Enone ratio (wt:wt)	0.23
Enone to Hydrocarbon Fuel (kg/kg)	0.94

A700: Lignin Conditioning and Deconstruction	
A700 RL composition	
Total Flow	22221.7
LIGNIN (wt% total mass)	30.69%
Cellulose (wt% total mass)	4.67%
Xylan (wt% total mass)	0.77%
Arabinan (wt% total mass)	0.07%
LgnSol (wt% total mass)	0.00%
Solids Flow (kg/hr)	14013.67
A700 BL composition	
Total Flow	92912.1
LIGNIN (wt% total mass)	6.64%
Cellulose (wt% total mass)	0.63%
Xylan (wt% total mass)	1.75%
Arabinan (wt% total mass)	0.64%
LgnSol (wt% total mass)	0.00%
Glucose (wt% total mass)	0.00%
Xylose (wt% total mass)	0.00%
Arabinose (wt% total mass)	0.00%
Sucrose (wt% total mass)	0.35%
Extract (wt% total mass)	13.14%
Acetic Acid (wt% total mass)	1.62%
Solids Flow (kg/hr)	11668.91
BL-to BCD	92912.05
BL-to ferm	0.014800
A700 BCD combined feed	
Total Flow	115133.7
LIGNIN (wt% total mass)	11.28%
Cellulose (wt% total mass)	0.90%
Xylan (wt% total mass)	0.15%
Arabinan (wt% total mass)	0.01%
LgnSol (wt% total mass)	0.00%
Glucose (wt% total mass)	0.81%
Xylose (wt% total mass)	1.74%
Arabinose (wt% total mass)	0.60%
Sucrose (wt% total mass)	0.28%
Extract (wt% total mass)	10.60%
Acetic Acid (wt% total mass)	1.31%
Solids Flow (kg/hr)	22876.25
Lignin Conditioning and Conversion	
Temperature	120.00
Pressure (atm)	5.00
NaOH Titer	58.07980769
A700 BCD pulp-outlet	
Total Flow	115133.7
LIGNIN (wt% total mass)	5.27%
Cellulose (wt% total mass)	0.47%
Xylan (wt% total mass)	0.08%
Arabinan (wt% total mass)	0.01%
LgnSol (wt% total mass)	6.02%
Glucose (wt% total mass)	1.29%
Xylose (wt% total mass)	1.82%
Arabinose (wt% total mass)	0.61%
Sucrose (wt% total mass)	0.28%
Extract (wt% total mass)	10.60%
Acetic Acid (wt% total mass)	1.31%
Solids Flow (kg/hr)	14564.61
BCD-SLS	
solids flow (kg/hr)	14564.61
entrained water in solids (kg/hr)	14564.61
liquid flow (kg/hr)	86004.50
Solubilization (across BCD)	
Cellulose	47.99%
Xylan	47.99%
Arabinan	47.99%
Lignin	53.33%
APL correction reactions	
Cellulose (wt % conversion)	100.00%
Cellulose (wt % degradation)	0.00%
Xylan (wt % conversion)	100.00%
Xylan (wt % degradation)	0.00%
Arabinan (wt % conversion)	100.00%
Arabinan (wt % degradation)	0.00%
Lignin (wt % conversion)	0.00%

A700: Muconic Acid Fermentation	
Production Feed Titer(s) (across average of all)	
Glucose	8.8
Xylose	12.4
Arabinose	4.1
Sucrose	2.1
Acetic Acid	9.9
Soluble Lignin	45.4
Extract	79.9
NaOH	38.2
Utilization (across average of all)	
Glucose	98.00%
Xylose	98.00%
Arabinose	98.00%
Sucrose	98.00%
Acetic Acid	98.01%
Soluble Lignin	98.00%
Extract	98.00%
Production broth Titer(s) (across average of all)	
Muconic Acid	68.53
OLEYEAST	37.6
ZYMO	1.00
Total DCW	38.61
NaOH	37.2
Clarification	
Ultrafilter Muconic Loss	4.0%
A700: Adipic Acid Upgrading	
Crystallization 1	
Muconic Crystallization Temperature	15.00
Muconic Acid recovery	98.7%
Hydrogenation	
Ethanol:Muconic Loading	4.00
Hydrogenation Temperature	78.00
Hydrogenation Pressure (PSI)	583.00
H2:Muconic Ratio (mol/mol)	2.673
Crystallization 2	
Adipic Crystallization Temperature	15.00
Adipic Acid single pass recovery	73.4%
Waste Water Treatment	
Hydraulic Load (L/hr)	445024.4
Hydraulic Load (gpm)	1959.4
Hydraulic Load (MMgal/day)	2.8
Total COD (kg/hr)	4148.8
Total COD (g/L)	9.3
NH3-N in Combined WW mg/L	66.2
Total BOD (KG/HR)	2987.1
Total BOD (g/L)	6.7
NH3-N DEMAND (mg/L)	-1.0
NH3-N ADDITION (KG/HR)	0.0
TOTAL Polymer (kg/hr)	0.0

BDO Pathway

Final Fuel Product	
Fuel Mass flow (kg/hr)	11031.6
Estimated Density (kg/L)	0.7
Fuel Volume Flow (L/hr)	15751.5
Fuel LHV (Mmkcal/hr)	116.1
Annual Fuel Volume (MM Gal/yr)	32.8
Annual Fuel GGE (MM GGE/yr)	31.3

A100: Feedstock	
Moisture Content	20%
Composition (wt% Dry Feed)	
Cellulose	35.0%
Xylan	19.5%
Arabinan	2.4%
Sucrose	0.8%
Lignin	15.8%
Acetate	1.8%
Extract	14.6%
Ash	4.9%
Mannan	0.6%
Galactan	1.4%
Protein	3.1%
Hydrolysis Mass yield (g/g biopolymer)	
Cellulose to glucose	1.111109
Xylan to xylose	1.136361
Arabinan to arabinose	1.136361

A200: Deacetylation & Pretreatment	
Deacetylation Conditions	
Temperature (C)	90
Pressure (atm)	1
NaOH loading (mg/L)	70
Solubilization to the Black Liquor	
Acetate	100%
Lignin	47.0%
Cellulose	2.0%
Xylan	10.0%
Arabinan	30.0%

A300: Whole Slurry Hydrolysis	
Operating Conditions	
Enzyme Loading	9.96
Hydrolysis	
Cellulose conversion	91.2%
Xylan conversion	90.0%
Arabinan conversion	85.0%
Residence times (hrs)	
Continuous saccharification	24
Batch saccharification	96
Batch fermentation	36

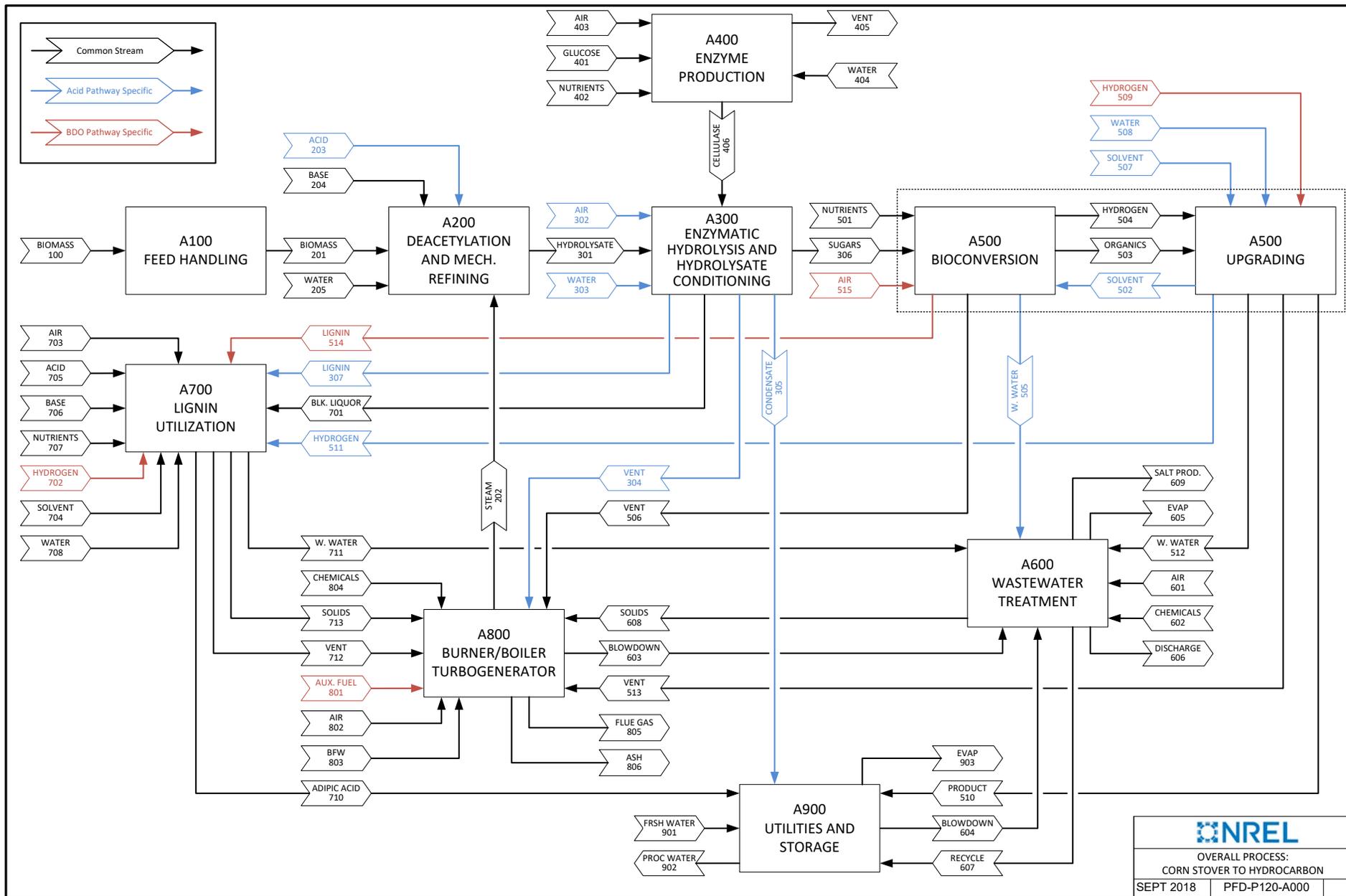
A500: BDO Fermentation	
2,3,BDO Titer broth	102.078175
Contamination Sugar Loss	3.0%
Utilization	
Glucose	98.1%
Xylose	92.5%
Arabinose	89.0%
Sucrose	95.0%
Diversion of substrate to Biomass (% of substrate Utilized)	
Glucose	2.040%
Xylose	2.053%
Arabinose	2.134%
Sucrose	0.000%
Diversion of substrate to 2,3-BDO (% of substrate Utilized)	
Glucose	96.88%
Xylose	97.26%
Arabinose	95.46%
Sucrose	100.00%
Maximum theoretical metabolic yield (g/g)	
Glucose to 2,3-BDO	0.500
Glucose to Biomass	0.820
Xylose to 2,3-BDO	0.500
Xylose to Biomass	0.820
Arabinose to 2,3-BDO	0.500
Arabinose to Biomass	0.820
Sucrose to 2,3-BDO	0.527
Sucrose to Biomass	0.863
Net Metabolic Yield (g/g substrate consumed)	
Glucose to 2,3-BDO	0.4846
Glucose to Biomass	0.0167
Xylose to 2,3-BDO	0.4866
Xylose to Biomass	0.0168
Arabinose to 2,3-BDO	0.4776
Arabinose to Biomass	0.0175
Sucrose to 2,3-BDO	0.5266
Sucrose to Biomass	0.0000
Solid Liquid Separation	
2,3,BDO recovery (% feed)	96.42%
A500: 2,3-BDO Upgrading	
Theoretical Yields , Fuel upgading	
2,3-BDO Dehydration (g butene/g BDO)	0.62257828
Butene Oligomerization (g Oligomer/g Butene)	1
Oligomer hydrogenation (g Hydrocarbon/g Oligomer)	1.0359

A700: Lignin Conditioning and Deconstruction		A700: Muconic Acid Fermentation	
A700 RL composition		Production Feed Titer(s) (across average of all)	
Total Flow	24928.0	Glucose	11.9
LIGNIN (wt% total mass)	27.36%	Xylose	16.1
Cellulose (wt% total mass)	9.90%	Arabinose	4.8
Xylan (wt% total mass)	5.76%	Sucrose	2.1
Arabinan (wt% total mass)	0.82%	Acetic Acid	10.1
LgnSol (wt% total mass)	0.00%	Soluble Lignin	46.3
Solids Flow (kg/hr)	17822.45	Extract	81.5
A700 BL composition		NaOH	38.9
Total Flow	92912.1	Utilization (across average of all)	
LIGNIN (wt% total mass)	6.64%	Glucose	98.00%
Cellulose (wt% total mass)	0.63%	Xylose	98.00%
Xylan (wt% total mass)	1.75%	Arabinose	98.00%
Arabinan (wt% total mass)	0.64%	Sucrose	98.00%
LgnSol (wt% total mass)	0.00%	Acetic Acid	98.01%
Glucose (wt% total mass)	0.00%	Soluble Lignin	98.00%
Xylose (wt% total mass)	0.00%	Extract	98.00%
Arabinose (wt% total mass)	0.00%	Production broth Titer(s) (across average of all)	
Sucrose (wt% total mass)	0.35%	Muconic Acid	71.85
Extract (wt% total mass)	13.14%	OLEYEAST	40.4
Acetic Acid (wt% total mass)	1.62%	ZYMO	1.29
Solids Flow (kg/hr)	11668.91	Total DCW	41.69
BL-to BCD		NaOH	38.9
BL-to BCD	92912.05	Clarification	
BL-to ferm	0.014800	Ultrafilter Muconic Loss	4.3%
A700 BCD combined feed		A700: Adipic Acid Upgrading	
Total Flow	117840.1	Crystallization 1	
LIGNIN (wt% total mass)	11.03%	Muconic Crystallization Temperature	15.00
Cellulose (wt% total mass)	2.09%	Muconic Acid recovery	98.8%
Xylan (wt% total mass)	1.22%	Hydrogenation	
Arabinan (wt% total mass)	0.17%	Ethanol:Muconic Loading	4.00
LgnSol (wt% total mass)	0.00%	Hydrogenation Temperature	78.00
Glucose (wt% total mass)	0.57%	Hydrogenation Pressure (PSI)	583.00
Xylose (wt% total mass)	1.60%	H2:Muconic Ratio (mol/mol)	2.654
Arabinose (wt% total mass)	0.58%	Crystallization 2	
Sucrose (wt% total mass)	0.27%	Adipic Crystallization Temperature	15.00
Extract (wt% total mass)	10.36%	Adipic Acid single pass recovery	73.4%
Acetic Acid (wt% total mass)	1.28%	Waste Water Treatment	
Solids Flow (kg/hr)	26685.02	Hydraulic Load (L/hr)	345223.5
Lignin Conditioning and Conversion		Hydraulic Load (gpm)	1520.0
Temperature	120.00	Hydraulic Load (MMgal/day)	2.2
Pressure (atm)	5.00	Total COD (kg/hr)	7128.1
NaOH Titer	57.83561938	Total COD (g/L)	20.6
A700 BCD pulp-outlet		NH3-N in Combined WW mg/L	37.8
Total Flow	117840.1	Total BOD (KG/HR)	4837.2
LIGNIN (wt% total mass)	5.15%	Total BOD (g/L)	14.0
Cellulose (wt% total mass)	1.09%	NH3-N DEMAND (mg/L)	107.5
Xylan (wt% total mass)	0.63%	NH3-N ADDITION (KG/HR)	29.4
Arabinan (wt% total mass)	0.09%	TOTAL Polymer (kg/hr)	1.6
LgnSol (wt% total mass)	5.88%		
Glucose (wt% total mass)	1.68%		
Xylose (wt% total mass)	2.27%		
Arabinose (wt% total mass)	0.67%		
Sucrose (wt% total mass)	0.27%		
Extract (wt% total mass)	10.36%		
Acetic Acid (wt% total mass)	1.28%		
Solids Flow (kg/hr)	16989.85		
BCD-SLS			
solids flow (kg/hr)	16989.85		
entrained water in solids (kg/hr)	16989.85		
liquid flow (kg/hr)	83860.37		
Solubilization (across BCD)			
Cellulose	47.99%		
Xylan	47.99%		
Arabinan	47.99%		
Lignin	53.33%		
APL correction reactions			
Cellulose (wt % conversion)	100.00%		
Cellulose (wt % degradation)	0.00%		
Xylan (wt % conversion)	100.00%		
Xylan (wt % degradation)	0.00%		
Arabinan (wt % conversion)	100.00%		
Arabinan (wt % degradation)	0.00%		
Lignin (wt % conversion)	0.00%		

Appendix D. Key Aspen Stream Data Tables

High-level stream table information from Aspen Plus modeling output follows, for key streams associated with each process operation area under both pathway scenarios. Space for stream tables was limited; below is a key to lumped components. As the stream table information focuses primarily on the high-level overall process and does not include every individual modeled stream within each process area, mass balance closure around a given unit area may not be 100%.

Other sugars (SS)	Arabinose, mannose, galactose, sucrose
Other organic acids (SS)	Acetic, butyric, muconic, and lactic acids, extractives
Fermentation nutrients (SS)	Sodium hydroxide, CSL, DAP, other minor nutrients
Other chemicals (SS)	Ammonia, ammonium sulfate, sodium sulfate, sodium nitrate
Solvent	TOA, toluene, ethanol
CO/SO _x /NO _x /H ₂ S	NO, NO ₂ , SO ₂ , CO, H ₂ S
Other structural carbohydrates (IS)	Xylan, arabinan, galactan, mannan
Protein (IS)	Corn protein, enzymes, denatured enzymes
Cell mass (IS)	Cell biomass for fermentation, enzyme, and wastewater organisms
Other insoluble solids (IS)	Ash, lime, calcium sulfate



Acids Pathway

ACIDS CASE		100	201	202	204	205	301	302	303	304	305	306	307	401	402	403	404	405	406	501	502	503	504	505	506	
Total Flow	kg/h	104,167	104,167	17,354	5,833	196,204	230,647	5,896	664,536	5,971	701,290	179,172	22,221	1,557	203	17,839	6,252	18,279	7,575	1,498	16,031	37,107	918	136,537	22,139	
Insoluble Solids	kg/h	70,483	70,483				57,306					286	14,014		24				398	327					3,558	
Soluble Solids	kg/h	12,850	12,850		5,833		321				0	48,521	457	1,324	123			0	30	514		21,076			2,065	9
Renewable hydrocarbon	kg/h																									
Adipic acid	kg/h																									
Water	kg/h	20,833	20,833	17,354		196,204	173,020		664,536	76	701,289	130,365	7,750	234	47	349	6,252	424	7,147	657					130,801	1,097
Glucose (SS)	kg/h											30,339	285	1,324												
Xylose (SS)	kg/h											16,291	153													
Other sugars (SS)	kg/h	642	642				321					1,862	18													178
Other organic acids (SS)	kg/h	12,208	12,208								0	22	0		23				22		324		21,076		1,647	9
Fermentation nutrients (SS)	kg/h				5,833										37						190					233
Sulfuric acid (SS)	kg/h																									
Other chemicals (SS)	kg/h										0	7	0		63			0	7							7
Soluble lignin	kg/h																									
Solvent	kg/h																					16,031	16,031			
Other organics	kg/h																									
Carbon dioxide	kg/h										0	0						1,304	0						113	20,974
Methane	kg/h																									
H2	kg/h																							918	1	48
O2	kg/h							1,373		1,373	0		0			4,074		3,135	0							11
N2	kg/h							4,523		4,522	0		1			13,416		13,416	0							
CO/SOx/NOx/H2S	kg/h														9											
Cellulose (IS)	kg/h	29,205	29,205				28,621					21	1,038													21
Other struct. carbohydr. (IS)	kg/h	19,948	19,948				17,725					38	1,845													38
Acetate (IS)	kg/h	1,508	1,508																							
Lignin (IS)	kg/h	13,132	13,132				6,960					139	6,821													139
Protein (IS)	kg/h	2,583	2,583				2,583					58	2,864		24				339	327						207
Cell mass (IS)	kg/h											1	58						59							3,125
Other insoluble solids (IS)	kg/h	4,108	4,108				1,417					28	1,389													28

ACIDS CASE		507	508	510	511	512	513	601	602	603	604	605	606	607	608	609	701	703	704	705	706	707	708	710	711	
Total Flow	kg/h	90	141,508	11,465	506	146,178	5,441	243,176	145	2,827	25,011	258,496	502	423,045	24,021	13,871	92,912	62,009	37	10,531	2,401	352	80,000	10,798	166,094	
Insoluble Solids	kg/h														10,710		11,669					70				6,285
Soluble Solids	kg/h								0			4	343		907	13,871	19,871			9,794	2,401	241				16,270
Renewable hydrocarbon	kg/h			11,442			0																			
Adipic acid	kg/h																									10,770
Water	kg/h		141,508	21		145,595	124	4,763	145	2,827	25,010	18,810	158	423,033	12,394		61,372	1,214		737		40	80,000		143,370	
Glucose (SS)	kg/h												0		1											27
Xylose (SS)	kg/h												0		1											38
Other sugars (SS)	kg/h											7			41		321									903
Other organic acids (SS)	kg/h											4	10		495		13,716					20			868	
Fermentation nutrients (SS)	kg/h								0				137		254		5,833				2,401	6				250
Sulfuric acid (SS)	kg/h																									
Other chemicals (SS)	kg/h											0	189		115	13,871				9,794			215			14,184
Soluble lignin	kg/h											0	1		6											139
Solvent	kg/h	90		2			87												37					28		
Other organics	kg/h					464	22					13		0	0											
Carbon dioxide	kg/h					118	5,146					5,047		3	4											24
Methane	kg/h																									
H2	kg/h			0	506		62						5													5
O2	kg/h							55,530			0	51,739		3	0			14,160								0
N2	kg/h							182,882			0	182,878		6	0			46,634								2
CO/SOx/NOx/H2S	kg/h																									
Cellulose (IS)	kg/h														21		584									
Other struct. carbohydr. (IS)	kg/h														38		2,222									
Acetate (IS)	kg/h																									
Lignin (IS)	kg/h														139		6,172									
Protein (IS)	kg/h														267								70			61
Cell mass (IS)	kg/h														10,216											6,224
Other insoluble solids (IS)	kg/h														28		2,691									

ACIDS CASE		712	713	802	803	804	805	806	901	902	903
Total Flow	kg/h	64,949	29,129	167,672	24,353	1,699	320,454	4,270	209,901	1,113,390	195,823
Insoluble Solids	kg/h		14,565			97		4,270			
Soluble Solids	kg/h	2				1,215	367				
Renewable hydrocarbon	kg/h										
Adipic acid	kg/h										
Water	kg/h	2,111	14,565	3,284	24,353	388	54,908		209,901	1,113,390	195,823
Glucose (SS)	kg/h										
Xylose (SS)	kg/h										
Other sugars (SS)	kg/h										
Other organic acids (SS)	kg/h	2									
Fermentation nutrients (SS)	kg/h						252				
Sulfuric acid (SS)	kg/h										
Other chemicals (SS)	kg/h					1,215	115				
Soluble lignin	kg/h										
Solvent	kg/h	8									
Other organics	kg/h										
Carbon dioxide	kg/h	10,245					77,814				
Methane	kg/h										
H2	kg/h	204									
O2	kg/h	5,744		38,289			7,553				
N2	kg/h	46,633		126,100			179,231				
CO/SOx/NOx/H2S	kg/h						580				
Cellulose (IS)	kg/h		540								
Other struct. carbohydr. (IS)	kg/h		959								
Acetate (IS)	kg/h										
Lignin (IS)	kg/h		6,064								
Protein (IS)	kg/h		2,864								
Cell mass (IS)	kg/h		58								
Other insoluble solids (IS)	kg/h		4,080			97		4,270			

BDO Pathway

BDO CASE		100	201	202	204	205	301	306	401	402	403	404	405	406	501	503	504	506	509	510	512	513	514	515	601
Total Flow	kg/h	104,167	104,167	17,354	5,833	196,204	230,647	238,222	1,557	203	17,839	6,252	18,279	7,575	679	193,111	432	27,174	410	11,032	181,435	1,488	24,927	6,743	239,617
Insoluble Solids	kg/h	70,483	70,483				57,306	17,241		24				398	152	364					364		17,822		
Soluble Solids	kg/h	12,850	12,850		5,833		321	45,653	1,324	123			0	30	222	4,072						4,072		151	
Renewable hydrocarbon	kg/h																				10,964		811		
Adipic acid	kg/h																								
Water	kg/h	20,833	20,833	17,354		196,204	173,020	175,327	234	47	349	6,252	424	7,147	305	168,935		624		64	176,618	9	6,226		4,693
Glucose (SS)	kg/h							28,621	1,324							533						533		20	
Xylose (SS)	kg/h							14,978								1,069						1,069		40	
Other sugars (SS)	kg/h	642	642				321	2,024								507						507		19	
Other organic acids (SS)	kg/h	12,208	12,208					22		23				22	150	1,484						1,484		55	
Fermentation nutrients (SS)	kg/h				5,833					37					71	472						472		18	
Sulfuric acid (SS)	kg/h																								
Other chemicals (SS)	kg/h							7		63			0	7		7						7		0	
Soluble lignin	kg/h																								
Solvent	kg/h																								
Other organics	kg/h															19,604		1		3	245	461	727		
Carbon dioxide	kg/h							0					1,304	0		137		19,711			137		0		
Methane	kg/h																								
H2	kg/h															0	432	23	410				207		
O2	kg/h						0			4,074		3,135	0			0		1,643			0		0	1,571	54,718
N2	kg/h						0			13,416		13,416	0					5,172					1	5,172	180,206
CO/SOx/NOx/H2S	kg/h								9																
Cellulose (IS)	kg/h	29,205	29,205				28,621	2,519								50						50		2,468	
Other struct. carbohydr. (IS)	kg/h	19,948	19,948				17,725	3,364								67						67		3,297	
Acetate (IS)	kg/h	1,508	1,508																						
Lignin (IS)	kg/h	13,132	13,132				6,960	6,960								139						139		6,821	
Protein (IS)	kg/h	2,583	2,583				2,583	2,922		24				339	152	61						61		2,966	
Cell mass (IS)	kg/h							59						59		18						18		882	
Other insoluble solids (IS)	kg/h	4,108	4,108				1,417	1,417								28						28		1,389	

BDO CASE		602	603	604	605	606	607	608	609	701	702	703	704	705	706	707	708	710	711	712	713	801	802	803	804
Total Flow	kg/h	145	3,537	15,491	255,764	266	311,705	22,446	14,163	92,912	406	63,673	37	10,835	2,660	387	80,000	11,121	164,152	66,588	33,980	1,300	212,775	25,406	1,567
Insoluble Solids	kg/h							8,499		11,669						76				6,683		16,990			103
Soluble Solids	kg/h	0			3	178		1,148	14,163	19,871				10,076	2,660	260				16,869					1,054
Renewable hydrocarbon	kg/h																								
Adipic acid	kg/h																			11,092					
Water	kg/h	145	3,537	15,491	18,963	87	311,694	12,761		61,372		1,247		758		51	80,000		139,704	2,165	16,990		4,167	25,406	411
Glucose (SS)	kg/h					2		2												36					
Xylose (SS)	kg/h					3		2												48					
Other sugars (SS)	kg/h					4		39		321										918					
Other organic acids (SS)	kg/h				2	3		504		13,716						25				977	2				
Fermentation nutrients (SS)	kg/h	0			0	61		278		5,833					2,660	7				297					
Sulfuric acid (SS)	kg/h													10,076											
Other chemicals (SS)	kg/h				0	106		322	14,163							228				14,593					1,054
Soluble lignin	kg/h				0	0		6												139					
Solvent	kg/h												37							29					
Other organics	kg/h				2	0		31												727	0				
Carbon dioxide	kg/h				8,122		4	1												24	10,616				
Methane	kg/h																					1,300			
H2	kg/h				5						406									5	95				
O2	kg/h			0	48,443		2	0						14,540						0	5,817			48,588	
N2	kg/h		0	180,200			4	0					47,886							2	47,885			160,020	
CO/SOx/NOx/H2S	kg/h				25		0	0																	
Cellulose (IS)	kg/h							50		584														1,284	
Other struct. carbohydr. (IS)	kg/h							67		2,222														1,715	
Acetate (IS)	kg/h																								
Lignin (IS)	kg/h							139		6,172														6,064	
Protein (IS)	kg/h							70								76				64				2,966	
Cell mass (IS)	kg/h							8,144												6,619				882	
Other insoluble solids (IS)	kg/h							28		2,691															103

BDO CASE		805	806	901	902	903
Total Flow	kg/h	367,036	4,279	133,396	308,422	121,177
Insoluble Solids	kg/h		4,279			
Soluble Solids	kg/h	599				
Renewable hydrocarbon	kg/h					
Adipic acid	kg/h					
Water	kg/h	62,839		133,396	308,422	121,177
Glucose (SS)	kg/h					
Xylose (SS)	kg/h					
Other sugars (SS)	kg/h					
Other organic acids (SS)	kg/h					
Fermentation nutrients (SS)	kg/h	277				
Sulfuric acid (SS)	kg/h					
Other chemicals (SS)	kg/h	322				
Soluble lignin	kg/h					
Solvent	kg/h					
Other organics	kg/h					
Carbon dioxide	kg/h	78,971				
Methane	kg/h					
H2	kg/h					
O2	kg/h	9,324				
N2	kg/h	214,782				
CO/SOx/NOx/H2S	kg/h	521				
Cellulose (IS)	kg/h					
Other struct. carbohydr. (IS)	kg/h					
Acetate (IS)	kg/h					
Lignin (IS)	kg/h					
Protein (IS)	kg/h					
Cell mass (IS)	kg/h					
Other insoluble solids (IS)	kg/h		4,279			