



Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2019 State of Technology and Future Research

Ryan Davis, Andrew Bartling, and Ling Tao

**NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC**

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

Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-76567
April 2020



Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2019 State of Technology and Future Research

Ryan Davis, Andrew Bartling, and Ling Tao

Suggested Citation

Davis, Ryan, Andrew Bartling, and Ling Tao. 2020. *Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2019 State of Technology and Future Research*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-76567.
<https://www.nrel.gov/docs/fy20osti/76567.pdf>

**NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy
Operated by the Alliance for Sustainable Energy, LLC**

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

Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-76567
April 2020

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

NOTICE

This work was authored 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.

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

U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free via www.OSTI.gov.

Cover Photos by Dennis Schroeder: (clockwise, left to right) NREL 51934, NREL 45897, NREL 42160, NREL 45891, NREL 48097, NREL 46526.

NREL prints on paper that contains recycled content.

Acknowledgments

The authors wish to thank the following researchers for their contributions to this work: Rick Elander, Nancy Dowe, Davinia Salvachua, Gregg Beckham, Derek Vardon, Eric Karp, Patrick Saboe, Mel Tucker, Xiaowen Chen, Min Zhang, Mike Himmel, Jeff Linger, Bruno Klein and Zia Abdullah from the National Renewable Energy Laboratory (NREL); David Thompson and Mohammad Roni from Idaho National Laboratory (INL), and Zhenglong Li from Oak Ridge National Laboratory (ORNL). This report provides a high-level overview of research data across key unit operations as utilized in updating NREL's State of Technology (SOT) benchmark models, based on inputs furnished from those researchers; however, it is not intended to present an exhaustive summary of all research activities, methods, or data outputs, and we defer to those and others' research works for further context.

List of Acronyms

AD	anaerobic digestion
ANL	Argonne National Laboratory
BCD	base catalyzed deconstruction (of lignin)
BDO	2,3-butanediol
BETO	Bioenergy Technologies Office
CEH	continuous enzymatic hydrolysis
CHP	combined heat and power
COD	chemical oxygen demand
CUBI	catalytic upgrading of biochemical intermediates (under ChemCatBio Consortium)
DDA	deacetylation and dilute acid (pretreatment)
DMR	deacetylation and mechanical refining (pretreatment)
EEO	Enzyme Engineering and Optimization (NREL research project)
EH	enzymatic hydrolysis
FCIC	Feedstock Conversion Interface Consortium
GGE	gallon gasoline equivalent
HDO	hydrodeoxygenation
INL	Idaho National Laboratory
IS	insoluble solids
LCA	life cycle assessment
LHV	lower heating value
LTAD	Low-Temperature Advanced Deconstruction (NREL research project)
MEK	methyl ethyl ketone
MFSP	minimum fuel selling price
MVR	mechanical vapor recompression
NREL	National Renewable Energy Laboratory
ORNL	Oak Ridge National Laboratory
SLS	solid-liquid separations
SOT	state of technology
TEA	techno-economic analysis
TS	total solids
TOPO	tri-octyl-phosphene-oxide
WHSV	weight hourly space velocity
WWT	wastewater treatment

Executive Summary

The annual State of Technology (SOT) assessment is an essential activity for biochemical platform research. It allows the impact of research progress (both directly achieved in-house at NREL and indirectly extrapolated from available public data) to be quantified in terms of economic improvements in the overall cellulosic biofuel production process for a particular conversion pathway. As such, initial benchmarks can be established for currently demonstrated performance and progress can be tracked towards out-year goals to ultimately demonstrate cost-competitive cellulosic biofuel technology.

Building upon recent efforts to transition NREL's biochemical platform R&D work towards ultimate 2030 goals to demonstrate less than \$2.50/gallon gasoline equivalent (GGE) fuel selling prices, experimental and techno-economic analysis (TEA) activities have primarily focused on "advanced" biochemical processing strategies to fuels and coproducts, guided by TEA modeling to highlight key barriers and priorities towards achieving this goal across a number of potential bioconversion pathways. The purpose of the present effort is to benchmark the latest experimental developments for these pathways as quantified by modeled minimum fuel selling prices (MFSPs), as a measure of current status relative to those final targets. For this SOT, TEA models were run for two separate biological conversion pathways to fuels, based on available data for integrated biomass deconstruction and hydrolysate processing; namely carboxylic acids (primarily butyric acid) and diols (2,3-butanediol [BDO]), reflecting NREL's recently-published 2018 biochemical design report focused on those two pathways. The models were run across three scenarios for lignin utilization, namely combustion, conversion to coproducts based on "base case" performance with biomass hydrolysate, and conversion to coproducts based on "high" performance demonstrated with model lignin monomer components.

Key process parameters utilized in the 2019 SOT include experimentally measured values of 84% glucan conversion, 82% xylan conversion, and 55% arabinan conversion to monomeric sugars through saccharification at 12 mg/g enzyme loading, based on the latest deacetylation and mechanical refining (DMR) pretreatment and batch enzymatic hydrolysis parameters observed. A confounding factor in the 2019 SOT deconstruction operations was a switch to utilize a new, more recalcitrant, source of corn stover feedstock (Idaho National Laboratory [INL] Lot 14), which required more severe conditions (caustic loading) relative to prior historical efforts. While the increased severity sufficed to overcome the higher recalcitrance, it also initially caused unanticipated challenges in some downstream operations (namely BDO fermentation) due in part to higher sodium levels. Eventually, these challenges were also overcome, leading to quite favorable bioconversion performance for both pathways, utilizing over 95% glucose and 89% xylose sugars at fermentation process yields approaching or exceeding future 2030 targets (albeit still requiring improving arabinose utilization as well as fermentation productivities). This was coupled with encouraging catalytic upgrading data for both intermediate products to finished fuels/blend stocks at 100% conversions across nearly all steps evaluated experimentally. Based on the combination of these process parameter values, the 2019 SOT MFSPs are estimated to be \$7.79/GGE and \$8.20/GGE (\$5.67/GGE and \$5.90/GGE conversion-only costs excluding feedstock contributions) in 2016-dollars, for the BDO and acids pathways respectively, attributed to the "burn lignin" basis scenario. These MFSPs are based on a total hydrocarbon fuel yield of 38.5 and 35.3 GGE/ton dry biomass for the respective pathways. The 2018 feedstock cost as furnished by INL is \$81.37/dry ton (2016\$), including a dockage fee to adjust to a 5% ash-

equivalent basis for modeling purposes. These results translate to a reduction of \$1.23/GGE (14%) and \$2.20/GGE (21%) in overall MFSPs for the two respective pathways, driven primarily by the improved fuel train yields noted above coupled with higher fermentation productivities for both pathways (yield improvements were more substantial in the acids pathway due to higher xylose utilization as well as a higher C4:C2 acid ratio, with C4 acids preferred over C2 given higher recovery efficiencies and lower losses across upgrading).

The alternative SOT scenarios reflecting lignin conversion to coproducts indicated MFSP estimates of \$10.80/GGE and \$11.47/GGE for “base case” experimental lignin conversion performance on biomass hydrolysate (BDO and acids pathways respectively); this would hypothetically reduce to \$9.72/GGE and \$10.29/GGE for “high” lignin conversion performance as observed for model lignin monomers. These results indicate that the lignin-to-coproduct train remains not yet economically profitable relative to burning the lignin, given higher costs for producing the adipic acid coproduct than the amount of resulting coproduct revenue generated (attributed in turn to low lignin deconstruction/conversion yields and fermentation productivities). There were no general improvements achieved for the key lignin coproduct TEA parameters in 2019 relative to initial demonstrated levels in the 2018 SOT, thus highlighting this process area as a key priority moving forward for future focus in ultimately contributing to MFSP reductions towards 2030 goals.

Finally, this milestone reports on key process sustainability indicators for the biorefinery conversion models including mass and carbon yields to fuels and coproducts, water consumption, and facility power balances/natural gas demands. In keeping with recent practices, formal life cycle analysis (LCA) sustainability metrics such as greenhouse gas emissions or fossil energy consumption are not calculated here, but will be deferred to partners at Argonne National Laboratory (ANL).

Table ES-1. Summary of MFSPs and Fuel Yields for 2019 SOT Cases Compared to 2017-2018 SOT

	BDO 2017 SOT Burn Lignin	Acids 2017 SOT Burn Lignin	BDO 2018 SOT Burn (Base) [High]^a	Acids 2018 SOT Burn (Base) [High]^a	BDO 2019 SOT Burn (Base) [High]^a	Acids 2019 SOT Burn (Base) [High]^a
Minimum Fuel Selling Price (\$/GGE, 2016\$)	\$10.08	\$11.05	\$9.02 (\$12.81) [\$11.54]	\$10.40 (\$14.66) [\$13.16]	\$7.79 (\$10.80) [\$9.72]	\$8.20 (\$11.47) [\$10.29]
Feedstock Contribution (\$/GGE, 2016\$)	\$2.67	\$3.19	\$2.59	\$2.99	\$2.11	\$2.30
Conversion Contribution (\$/GGE, 2016\$)	\$7.41	\$7.86	\$6.43 (\$10.22) [\$8.95]	\$7.41 (\$11.67) [\$10.17]	\$5.67 (\$8.69) [\$7.61]	\$5.90 (\$9.17) [\$7.98]
Hydrocarbon Fuel Yield (GGE/dry ton)	31.4	26.3	32.3	28	38.5	35.3

^a (#) = “base case” lignin conversion on biomass hydrolysate; [#] = hypothetical “high” productivity w/ model lignin monomer compounds.

Table of Contents

Introduction	1
Discussion of Relevant Inputs Used in the SOT	3
Feedstock	6
Pretreatment and Enzymatic Hydrolysis	6
Post-Hydrolysis Clarification (Acids Pathway)	8
Bioconversion and Upgrading to Fuels	8
Lignin Utilization	11
Results	13
TEA Results	13
Sustainability Metric Indicators	22
Concluding Remarks	24
References	26
Appendix A. TEA Summary Sheets for 2019 SOT Benchmark Models (2016-dollars)	27
Appendix B. Life-Cycle Inventory (LCI) for 2019 SOT Benchmark Models	33

Introduction

The National Renewable Energy Laboratory (NREL) develops and maintains techno-economic models that describe the process and production economics of conceptual biochemical conversion pathways to biofuels and bioproducts. For a given set of conversion parameters, material and energy balance and flow rate information are generated using Aspen Plus process simulation software [1] assuming a feed rate to the biorefinery of 2,205 dry U.S. tons of biomass per day (2,000 metric tonne/day). These data are used to size and cost process equipment and compute raw material and other operating costs. Using a discounted cash flow rate of return analysis, the minimum fuel selling price (MFSP) required to obtain a net present value (NPV) of zero for a 10% internal rate of return (IRR) is determined. The result is a so-called techno-economic model that reasonably estimates an “ n^{th} -plant” production cost for this pre-commercial process.

Recently, the Biochemical Platform Analysis project published the 2018 Biochemical Design Report Update (hereafter referred to as the 2018 design report), which documented the details and assumptions behind a techno-economic analysis (TEA) model focused on highlighting future technical targets required for achieving a modeled n^{th} -plant MFSP of \$2.50/ gallon gasoline equivalent (GGE) or less by the year 2030 through biochemical processes [2]. Specifically, the report considered two separate pathways for biological and catalytic upgrading of lignocellulosic sugars to hydrocarbon fuels via carboxylic acid and diol intermediates, with associated upstream and downstream process integration considerations. These two pathways were selected among other bioconversion options being based on anaerobic fermentation, at considerable cost advantages relative to aerobic fermentation pathways (e.g. oleaginous yeast lipids) based on previously-demonstrated TEA findings summarized in a go/no-go decision milestone [3]. Both pathways included a deacetylation and mechanical refining (DMR) pretreatment step, followed by whole-slurry batch enzymatic hydrolysis in the diol case or by continuous enzymatic hydrolysis with integrated solid/liquid separations in the acids case, followed by fermentation and recovery of the intermediate molecule and subsequent catalytic upgrading to hydrocarbon fuels; both pathways also included supporting operations including wastewater treatment, waste solids/gas boiler and steam/power generation, and heating/cooling utilities. Finally, in order to ultimately achieve the MFSP targets below \$2.50/GGE, both pathways were shown to rely heavily on the inclusion of value-added coproducts (adipic acid as an example) from lignin and other residual biomass, requiring approximately 50% conversion of biomass lignin to adipic acid, in addition to utilization of biomass extractives, unconverted carbohydrates, and other components, in order to reach this ultimate cost target.

The purpose of this report is to summarize recent R&D progress based on 2019 experimental findings for the key process steps behind both of the design case pathways described above, and to quantify the resulting MFSPs in order to benchmark current state of technology (SOT) performance relative to the future design case targets. The intent of this report is *not* to provide an exhaustive documentation of all research activities pertaining to all steps under the above-noted pathways, and we defer to the associated reports of the Platform R&D projects for that information. Rather, this assessment focuses on quantifying the MFSP benchmarks attributed to the latest SOT performance for these pathways, based on experimental data currently available for an integrated process.

The annual SOT models follow an established practice in place since 2007 as a means to quantify the economic implications for observed experimental performance, by correlating experimental performance data for the various unit operations with modeled minimum fuel selling price on a dollar-per-GGE basis. This allows for both establishing cost benchmarks for a process pathway, as well as documenting progress moving beyond the initial benchmarks. With minimal changes to the unit operations in the Aspen Plus model, the projected conversions from the future target case are replaced by present conversions that have been (ideally) experimentally verified at the bench and/or pilot scale on process-relevant material. In cases where in-house experimental data does not yet exist, publicly available information such as that provided in published literature are occasionally utilized. By comparing the SOT year over year, research advances can be quantified in terms of their impact on overall biorefinery production economics to track progress towards final 2030 goals of \$2.50/GGE, as well as more near-term interim progress.

It should always be emphasized that our analyses and the resultant MFSP values carry some uncertainty related to the assumptions made about capital and raw material costs. Without a detailed understanding of the basis behind it, the absolute computed MFSP has limited relevance. MFSP values are therefore best used to compare technological variations or process improvements against one another. By demonstrating the cost impact of various process parameters individually or in concert, the model helps guide research by indicating where the largest opportunities for cost reduction exist. It is also acknowledged that “State of Technology” is arguably a misnomer since no commercial cellulosic hydrocarbon biofuel plants exist today (based on biological conversion technology or bioproduct co-processing strategies). Furthermore, this report is not intended to represent the “state of the industry” including commercial organizations who have been developing aspects of the technology privately, and who may be further ahead than what is presented in public literature or NREL data regarding parameters related to biological conversion performance of engineered organisms. The majority of the unit operation conversion yields in the SOT stem primarily from laboratory-scale data for enzymatic hydrolysis, hydrolysate clarification, and sugar/lignin bioconversion operations, with pretreatment done at pilot scale. There is of course some risk in assuming that bench-scale performance data is applicable at larger scale, and a key aspect of R&D efforts moving forward will be to scale operations up beyond bench-scale and otherwise pursue process integration operational strategies leading up to future demonstration targets.

Discussion of Relevant Inputs Used in the SOT

The two design case target pathways as evaluated in the 2018 design report are depicted schematically in Figure 1. In summary, the overarching process designs are based on deacetylation and mechanical refining (DMR) pretreatment of herbaceous biomass, followed by enzymatic saccharification, hydrolysate conditioning (sugar concentration, applicable in the acids pathway), and bioconversion to hydrocarbon intermediates, which are then subsequently catalytically upgraded to hydrocarbon fuels/blend stocks. Solubilized lignin from the DMR stage is combined alongside the residual lignin solids recovered downstream, and routed through base catalyzed deconstruction (BCD) to further break lignin polymers down to soluble oligomers, subsequently fermented to muconic acid (along with solubilized extractives and carbohydrates) which is then hydrogenated to adipic acid as a value-added coproduct.

The “deacetylation” step in DMR is modeled in the design case as a continuous counter-current alkaline extraction unit with a screw press to dewater extracted biomass, sending the pressed liquor back through the operation to further concentrate the black liquor and (as a target) somewhat mitigate loss of hemicellulose carbohydrates. In the acids case, the hydrolysis step is based on the newer continuous enzymatic hydrolysis (CEH) approach being investigated experimentally at NREL, utilizing a series of hydrolysis vessels each connected to microfilter/ultrafilter membranes to remove sugars and send solids/enzymes to the next stage. In the diols case (producing 2,3-butanediol [BDO]), the whole hydrolysate slurry is sent through fermentation, and solids are recovered afterwards in a lignin press, with the remaining aqueous BDO stream sent directly to catalytic upgrading. Both pathways include on-site wastewater treatment, albeit utilizing a simpler process without the need for anaerobic digestion (AD) in the target design cases given significantly lower chemical oxygen demand (COD) levels than prior designs. Finally, residual solids, wastewater sludge, and off-gas streams are combusted in a boiler connected to a steam turbine generator set to provide combined heat and power benefits to the facility.

Relative to the final design case targets to be achieved by 2030 for key operations as noted above, the processes evaluated in this SOT make a number of modifications based on current efforts (also reflected in Figure 1):

1. DMR step – deacetylation/alkaline extraction: While the future target asserts the use a continuous counter-current alkaline extraction unit as described above and in the design report, experimentally this step currently maintains standard batch deacetylation as was utilized in prior 2017-2018 SOTs.
2. Enzymatic hydrolysis – acids pathway: The new CEH concept is still in early stages of research, and not yet ready to be deployed to support this year’s SOT in an integrated process. Accordingly, the process reverts to standard batch hydrolysis (utilizing the same parameters as in the BDO pathway), followed by the flocculent-assisted vacuum filter press operation to perform in-line solid/liquid separations downstream of batch EH (and then to sugar concentration via evaporation as had also been utilized in the design case).
3. Fermentation – BDO pathway: While the design case assumes moving to fully anaerobic BDO fermentation by 2030 (with co-production of hydrogen to satisfy redox balances), this will require further strain engineering to accomplish moving forward. At present, the

SOT model maintains the use of minimal oxygen delivery via an air overlay in the headspace of the fermentor vessel, consistent with the experimental approach (no hydrogen co-production).

4. Fermentation – acids pathway: The design case assumed exclusive production of butyric acid to minimize recovery losses and maximize final carbon yields. The organism utilized in the present SOT has continued to improve on this aspect, moving from 90% butyric acid selectivity vs acetic acid in the 2018 SOT to 98% in the 2019 SOT, thus nearly achieving exclusive production of butyric acid. However, the small amount of acetic acid still remaining is captured across pertraction and processed through catalytic upgrading.
5. Lignin utilization: Similar to 2018 (when lignin conversion to coproducts was first incorporated to the SOTs), the present SOT again reflects three lignin utilization scenarios, given that lignin deconstruction and upgrading is still in an earlier stage of research than most other operations and the performance for this process train again translates to a higher cost penalty on overall MFSP than simply burning lignin. Both fuel pathways consider the following scenarios for lignin utilization:
 - A. Convert lignin under base case conversion parameters observed with actual lignin hydrolysates
 - B. Convert lignin under higher conversion parameters observed with pure model lignin monomer compounds
 - C. Route all lignin to the boiler to provide more consistent results for comparison with prior SOTs
 - i. In case #3 (burn lignin), the resulting COD concentration to the wastewater treatment (WWT) system increases as DMR liquor is routed directly to WWT rather than the coproduct train; accordingly, the WWT system reverts to the full set of operations as had been utilized in prior designs, namely again including the anaerobic digestion step at increased WWT system costs.

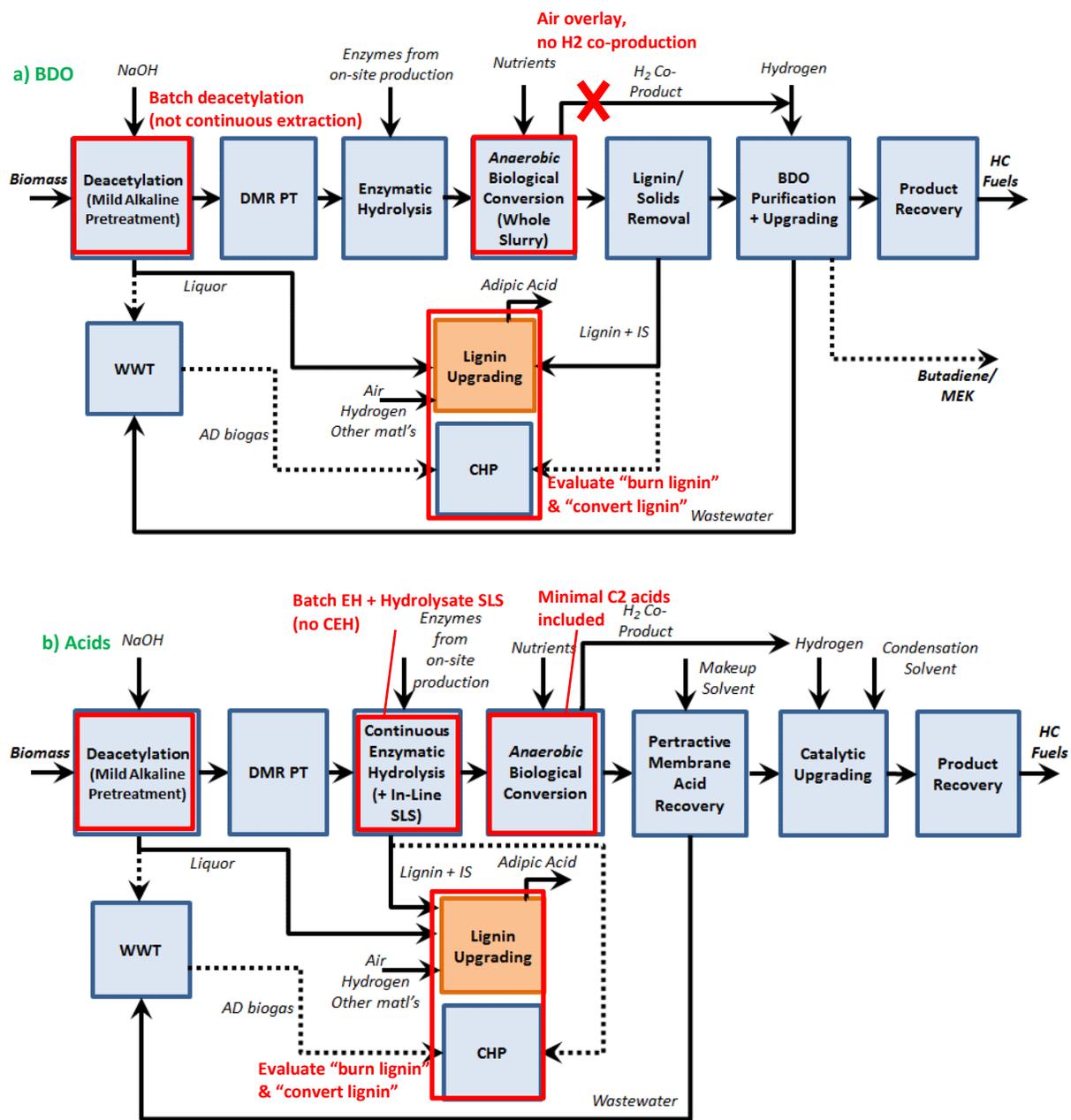


Figure 1. Block diagram schematics for 2030 "advanced process" configurations as projected in 2018 design report [2]. Modifications from the 2030 goals as reflected in current 2019 SOT are denoted in red.

Feedstock

Consistent with prior years, feedstock assumptions for the SOT between 2017 and 2019 are based on inputs provided annually by partners at Idaho National Laboratory (INL). Also similar to prior SOTs, as the primary focus of this work is to isolate the impacts of technology performance improvements strictly within the confines of the conversion process, this requires assuming a fixed biomass composition across all projected years to avoid artificial yield variances tied to varying feedstock compositions (i.e., ash content). INL's updated herbaceous feedstock cost guidelines allow for maintaining a fixed ash composition in the biorefinery conversion model, by way of valorizing ash variances using "dockage costs" on the feedstock side relative to the target 5% ash content (personal communication with Erin Searcy, INL, September 2015). Table 1 presents the resulting feedstock costs for a "5% ash-equivalent" feedstock, along with the underlying dockage fees associated with the variance from 5% for any given year (allowing us to keep ash and all other compositional details constant in our SOT models). These costs are largely consistent with those utilized in previous SOT assessments, but now updated to 2016-year dollars. All other feedstock components were set consistent with the compositional basis presented in our 2018 design report, including 59% total carbohydrates, 16% lignin, etc. [2, 4]. In the 2019 SOT, INL achieved a roughly 3% reduction in delivered feedstock cost relative to the 2018 basis, at \$81.37/dry ton inclusive of the above dockage adjustments [personal communication with David Thompson, INL, September 2019].

Table 1. Feedstock Costs Adjusted to 5% Ash for Years 2017-2019 (2016-year dollars; courtesy David Thompson and Mohammad Roni, INL)

	2017	2018	2019
Total feedstock cost to biorefinery at 5% ash equivalent (\$/dry ton)	\$83.90	\$83.67	\$81.37
Ash dockage vs 5% baseline (\$/dry ton) ^a	\$1.26	\$1.24	\$1.58

^a Ash dockage fee is included in the overall "cost to biorefinery" and accounts for variances in ash content above 5% projected by INL [personal communication with INL, Sept 2015-Sept 2019]

Pretreatment and Enzymatic Hydrolysis

Given the recent shift in focus towards including lignin deconstruction and conversion to coproducts in the integrated processes (as a key prerequisite to ultimately achieving \$2.50/GGE or even \$3/GGE goals in the future), this precludes the use of dilute acid pretreatment approaches and instead requires DMR in order to maintain convertible lignin throughout the process, while also enabling cleaner sugars with less salts and inhibitors. As noted above, while the DMR operation is ultimately projected to be performed with the use of a continuous counter-current alkaline extraction unit in order to better concentrate the black liquor components, conserve water, and mitigate hemicellulose solubilization losses[2], such an operation is not yet available at NREL to support SOT efforts and thus is not reflected in this exercise at present. A similar concept has been demonstrated experimentally through reverse-sequence batch recycling of black liquor [5], but this would incur a complex system of numerous batch reactors and holding tanks, which would not likely be economical for this process focused on commodity

fuels. Accordingly, the present SOT reverts to the more simplistic single-stage batch deacetylation operation as utilized in the prior 2017 and 2018 SOTs.

However, one key difference between the prior 2017-2018 and current 2019 SOTs is the basis feedstock processed through DMR-EH. In prior recent SOTs, NREL made use of a more convertible corn stover feedstock (INL Lot #13) for generating deconstruction data as well as the hydrolysate for others to use in downstream conversions. However, in 2019 NREL switched to a new source (INL Lot #14) which was seen to be significantly more recalcitrant to hydrolysis under prior SOT conditions for DMR pretreatment. Accordingly, in order to overcome this recalcitrance, more severe DMR conditions were employed in the 2019 SOT, namely a sodium hydroxide loading of 80 kg/dry tonne biomass (vs 70 kg/tonne previously), while maintaining a similar DMR temperature (90 °C vs 92 °C previously). Although the higher caustic loading is not ideal for overall economics, it was deemed necessary given earlier data suggesting that anything less than 80 kg/tonne would translate to low sugar yields generally below 60% in enzymatic hydrolysis. The more severe DMR conditions were shown to overcome the new biomass recalcitrance as well as to support good hydrolysis yields as discussed below (however, also as discussed later, the resultant increased sodium content was suspected to cause subsequent problems in BDO fermentation as well). At these conditions, the deacetylation (mild alkaline pretreatment) operation produced a black liquor product containing roughly 16% of the original biomass xylan, 2% of the glucan, 46% of the arabinan, 11% of the ash, and 80% of the acetates, along with solubilizing 50% of the biomass lignin. In the “convert lignin” scenarios for adipic acid co-production, this liquor stream is routed to the lignin coproduct train to be (partially) utilized for muconic/adipic acid. In the “burn lignin” SOT scenario, the liquor is routed to wastewater treatment which requires reverting back to the full WWT section including the anaerobic digestion step as originally designed in prior TEA models [4], [6]. The power for the mechanical refining step was set at 200 kWh/dry ton biomass, consistent with vendor inputs provided previously [7].

For the present SOT iteration, the pretreated solids from DMR are routed to standard batch enzymatic hydrolysis in both pathways (see discussion above). While new work is being conducted under NREL’s Enzyme Engineering and Optimization (EEO) research project in conjunction with industry to develop more tailored enzymes to DMR substrates, that work is still in early stages of development and data from NREL’s Low-Temperature Advanced Deconstruction (LTAD) project utilizing commercial enzyme packages through pilot scale deconstruction operations is maintained in this SOT. Under the LTAD work, the elevated severity conditions for DMR were shown to achieve good hydrolysis performance, namely 84% glucose and 82% xylan yields (with additional yields to glucose/xylose oligomers of 8% and 14% respectively), although with slightly lower arabinose yields of 55%, all based on a total enzyme loading of 12 mg/g cellulose (90:10 blend of cellulase and hemicellulase enzymes) carried out at 20% total solids for 5 days [8].

Beyond the base case DMR-EH conditions and results summarized above, another new approach that was investigated by the LTAD project in 2019 was the addition of ozone treatment between deacetylation and mechanical refining [8]. That work found promising potential for the addition of ozone treatment, achieving up to 93% yields of both glucose and xylose at 12 mg/g enzyme loading or alternatively 88% glucose and 90% xylose yields at 10 mg/g enzyme loading (final 2030 design case targets are 90% yields at 10 mg/g enzyme loading). While those preliminary

results are encouraging, given the early state of understanding for such a process option, including uncertainties around ozone generation or purchase costs for TEA modeling, ozone treatment is not yet a part of the formal SOT process framework this year. Moving forward, if such uncertainties could be reduced as more details become available, ozone treatment may be reflected in future SOTs, i.e. at least as a temporary measure to further improve enzymatic hydrolysis performance on DMR substrates (with a potential longer-term solution focused on DMR-tailored enzymes without needing this additional step).

Post-Hydrolysis Clarification (Acids Pathway)

For the acids pathway, following batch EH, the hydrolysate is sent through a solid/liquid separation unit (vacuum filter belt) to remove lignin and other residual insoluble solids as required for downstream bioreactor operation; this step is not required for the BDO pathway as 2019 BDO fermentation data was based on processing whole slurry rather than clarified sugars. All parameters for the vacuum belt filtration step are maintained consistently with those utilized in prior recent SOTs. As documented previously, recent experimental work with vacuum belt filtration has established that this is a challenging operation when placed downstream of the EH step given more fine and less filterable particles present in this location. Accordingly, sugar retention has been demonstrated at 95% (5% loss to the solids product), which is not envisioned to be increased significantly moving forward and the same 95% basis is maintained here. Additionally, this occurs using a water wash to assist with sugar retention, set at a wash ratio of 17.5 L/kg insoluble solids (IS), filter capacity of 12 kg IS/m²h, and assistance of a flocculant (branched polyamide with cationic charges) which is utilized at a loading of 20 g/kg IS, consistent with prior benchmarks for this operation with DMR-pretreated hydrolysate (which is considerably more challenging to filter than deacetylation and dilute acid (DDA)-pretreated hydrolysate, and the operational parameters reflect this accordingly) [9]. Moving forward, once CEH is ready to be implemented in future SOTs, the vacuum filtration operation will be removed given that solid/liquid separation occurs as an integral aspect of CEH with the included microfiltration/ultrafiltration membrane steps (although further solids concentration will still make use of a lower-cost lignin press on the residual solids outlet stream).

Bioconversion and Upgrading to Fuels

In the acids pathway, the clarified hydrolysate is routed to sugar concentration (not currently included as a critical parameter for demonstration based on standard technology), and then to bioconversion. The clarified and concentrated hydrolysate undergoes anaerobic fermentation to convert sugars to mostly butyric acid, with a minimal amount of acetic acid co-produced at a roughly 50:1 mass ratio (less than 2 wt% acetic acid) using *Clostridium tyrobutyricum*. This represents a continued improvement over the 2018 SOT which achieved a 9:1 ratio of the C4 vs. C2 acids in the same organism, as well as the 2017 SOT which utilized *C. butyricum* that yielded a 3:1 ratio (acetic acid incurs significantly higher losses than butyric acid both across recovery as well as upgrading and phase separation). Similar to the 2018 SOT, this was achieved under a more optimal pH of 5, which facilitates better pertractive recovery of the acids while still providing a suitable environment for fermentation relative to earlier SOTs conducted at pH over 6 (as reiterated in the 2017 SOT and prior TEA milestones, pertractive recovery of the acids or an alternative approach will be key to maintaining economic viability compared to pH-controlled fermentation with significant amounts of added caustic and subsequent salt disposal costs). In contrast to prior SOT experimental efforts which generally performed acid fermentation in batch

mode with separate operations to demonstrate fermentation and pertractive acid recovery in isolation, this year's 2019 SOT effort was done in a physically integrated system, with fermentation operated in fed-batch mode, coupled with continuous recovery of acids across a pertraction membrane. Under that setup, optimal sugar feeding strategies are not yet well-understood, and a decision was made to keep glucose concentrations low in order to promote high xylose consumption, completing the fermentation cycle with some remaining hemicellulose sugars. In particular, the remaining xylose was not a reflection of a biological ability or limitation to effectively utilize those sugars, but rather a reflection of the fermentation feeding/operating strategy, where either (a) sugar feeding could have been stopped sooner to allow the organism to more completely consume xylose, or (b) remaining unconverted sugars could be used as part of the initial fed-batch substrate. Accordingly, the conversion of sugars to products was set at 95% glucose (demonstrated), 95% xylose (not fully demonstrated, but dictated by operational decisions noted above), and 20% arabinose; with an additional 2.5% conversion to cell biomass for glucose/xylose and 9% for arabinose. The TEA implications on experimentally measured xylose utilization as reflected at the end of the fermentation run (70% overall, with 67% converted to acids) are also reported below. Fermentation productivity was 0.62 g/L-hr, roughly double that of the 2018 SOT basis at 0.3 g/L-hr.

Recovery of acids was observed to be 98.4% and 76.4% for butyric and acetic acids respectively, based on a solvent system comprised of 20% tri-octyl-phosphene-oxide (TOPO) plus 40% undecanone in mineral oil. Experimentally, the acids were subsequently recovered from the solvent using 4 N sodium hydroxide as a stripping agent to facilitate *in vivo* fermentation studies at bench scale, but this recovery is performed in the optimized TEA model with distillation to boil the acids off from the heavier-boiling solvents. These parameters also represent an improvement over the 2018 recoveries at 60% C2 and 95% C4 acids. The recovered acids are next subjected to catalytic upgrading, based on data furnished by NREL researchers under the ChemCatBio catalytic upgrading of biochemical intermediates (CUBI) efforts.

Catalytic upgrading of the pertractive acid products largely remains consistent with prior 2018 data, which has focused exclusively on butyric acid (now more in line with the latest 2019 fermentation data producing minimal acetic acid). In summary, acid substrate first undergoes ketonization over a ZrO_2 catalyst at 4 hr^{-1} weight hourly space velocity (WHSV), achieving 100% acid conversion with 93% selectivity to 4-heptanone; the remaining 7% represents unknown ketones, but given experimental indications that this fraction follows a similar fate as 4-heptanone producing fuel grade hydrocarbons, the TEA model assumes complete conversion to the 4-heptanone component. The small amount of residual acetic acid reacts completely with 45% converted to acetone and 55% to 2-pentanone. Relative to the 2018 SOT model, which had utilized a temperature of 365°C , the primary update this year reflects a higher ketonization temperature of 435°C in keeping with the latest experimental understanding for a realistic/optimal condition for this step. The intermediate ketone stream is purified and routed to condensation to produce a mixture of C9-C15 oxygenated ketones/enones. All ketone condensation parameters remain unchanged from 2018, including use of a slurry reactor utilizing a Nb_2O_5 catalyst at a ratio of 1:4 wt catalyst:ketone, 10 hour residence time, and requirement for toluene solvent at a loading of 4:1 wt toluene:ketone. Operating pressure and temperature were 150 psig and 180°C respectively. Resulting per-pass conversion of 4-heptanone was 40% with a 90% selectivity to C14-enone (again with the remaining 10% of unknown product behaving similarly to C14-enone through downstream conversion to hydrocarbon, thus the model assumes

only C14-enone), along with 100% conversion of any acetone/2-pentanone to C8-C11 enones, resulting in an overall process yield of 92 wt% to enone products from feed ketones. Finally, the enone intermediates are upgraded to hydrocarbons via hydrodeoxygenation (HDO), again largely maintaining consistent details as the prior 2018 SOT including use of a 3%Pt/Al₂O₃ catalyst at a WHSV of 4.7 hr⁻¹ achieving 100% conversion to products (primarily C14 branched hydrocarbon from the C14-enone). Compared to the 2018 operating conditions of 500 psig and 270°C, 2019 experimental learnings have found a more realistic/optimal temperature to be 334°C, thus this higher temperature was incorporated here.

For the BDO pathway, whole slurry fermentation was initially attempted on the new 2019 DMR-EH hydrolysate using a strain of *Zymomonas* engineered to utilize arabinose. However, this fermentation experienced significant inhibition, hypothesized to be tied to a combination of elevated sodium levels (reflecting the more severe DMR conditions/NaOH loadings required to overcome the higher feed lot recalcitrance noted above) as well as too high initial concentration of sugars for a batch fermentation due to the more easily digested feedstock from more severe deacetylation conditions. Although not helpful for supporting SOT efforts focused on demonstrating performance improvements, this observation provides an example case study supporting the importance of current Feedstock Conversion Interface Consortium (FCIC) efforts to understand exactly these types of interactions between feedstock variability and impacts on conversion conditions/yields; thus, this type of data will prove valuable in leveraging under future FCIC activities. However, in order to achieve the key priority for demonstrating SOT benchmark improvements in the present exercise, the BDO fermentation experiments were re-run utilizing the 2018 SOT *Zymomonas* strain (considered to be more robust, but without arabinose utilization capabilities), and after diluting the hydrolysate to approximately 150 g/L sugars (based on predicted sugar concentration levels calculated in the Aspen models before receiving deacetylation mass balance data). Upon subsequently receiving deacetylation liquor mass balance information, the model confirmed a resultant sugar concentration very near 150 g/L, validating that the adjusted sugar concentrations were appropriate.

This second experimental fermentation run was more successful, achieving nearly 100% overall glucose utilization and 92% xylose utilization at 97% metabolic yield to BDO (albeit no arabinose utilization) within 48 hours (roughly 1.4 g/L-hr productivity, a 30% improvement over 2018). Moreover, with the fermentation process being based on whole slurry, the retention of enzymes from upstream EH promoted an additional 7.1% yield of glucose and 2.0% of xylose from available oligomers relative to initial starting monomeric sugars. In all, from a combined glucose plus xylose concentration of 150 g/L (including oligomer conversion), experimental BDO titer reached 69 g/L compared with 54 g/L BDO in 2018 – and approximately 90% of theoretical process yield from total available sugars. Acetoin byproduct yield was negligible, at 0.3% wt% of total BDO + acetoin production. These parameters are attributed to bench-scale experimental work done in a stirred 0.5L batch reactor with an air overlay (air delivered to the headspace of the CSTR), rather than with dedicated air sparging into the broth, to demonstrate proof-of-concept that oxygen requirements for this pathway are minimal (limited strictly to satisfying redox balances) such that the process could be commercially implemented utilizing anaerobic fermentation equipment (i.e. large 1-MM gal stirred-tank reactors, rather than smaller/costlier aerated bubble columns with air compression). Additionally, NREL researchers are working to evaluate alternative means of balancing cell redox demands that do not involve any oxygen, thus mitigating this issue in the future.

For BDO catalytic upgrading, experimental data observed by Oak Ridge National Laboratory (ORNL) collaborators were applied in the TEA models, converting 2,3-BDO to hydrocarbon intermediates over copper-based zeolite catalysts (Cu/PMFI) at 200°C-250°C. The fermentation broth was clarified by filtrations. In the SOT modeling, the fermenter broth is first clarified in a lignin press (consistent with that used in prior ethanol work) and then sent to BDO polishing filtration, assumed to be two parallel skid units made up of microfiltration, nanofiltration and ion exchange, including clean-in-place systems and backwash. The ion exchange system uses a separate-bed configuration, with strong acid cation and weak base anion resins. The products from BDO catalytic upgrading were a mixture of butenes, propene, C5+ olefins and methyl ethyl ketone (MEK). In the SOT models, 100% of the BDO is converted at 220°C based on inputs from ORNL for BDO upgrading performance. Hydrogen is added to the reactors at a hydrogen-to-BDO ratio of 7.2 (molar basis). The catalyst is costed at a WHSV of 1.0 hr⁻¹ (per guidance from ORNL researchers based on the latest bench scale experimental data) with assumed annual catalyst replacement. The product mixture is then purified by simple distillation before subsequent oligomerization reactions of the olefin mixture to olefin oligomers. The oligomers (generally C₄-C₂₀ olefins) are then hydrotreated to hydrocarbon fuels. All reactor design and cost assumptions are consistent with the details presented in the 2018 design report update [2].

Lignin Utilization

In both pathway options, residual solids exiting hydrolysis (acids) or fermentation (BDO) and the DMR black liquor stream are processed further to allow economic valorization of the remaining lignin carbon. First the streams are conditioned as needed to release lignin monomers and clarify the slurries of suspended solids. The clarified/conditioned lignin streams are fed to aerobic fermentation where muconic acid is produced from lignin monomers, purified, and upgraded to adipic acid for sale as a polymer grade product. For the SOT models the black liquor is sent directly to fermentation without further conditioning or clarifying (based on the approach taken experimentally). The residual hydrolysis solids undergo base catalyzed deconstruction at conditions of 120 °C solubilizing 85% of the solids. Bench scale results show degradation of carbohydrates in both the black liquor stream and the BCD liquor which is modeled in the SOT as conversion to short chain acids (e.g., lactic acid).

Relative to the 2018 SOT, there were no substantial changes in 2019 with respect to either lignin deconstruction to convertible species, or to fermentation performance based on actual hydrolysate. Muconic acid titer was improved in 2019 based on an alternative scenario utilizing model lignin monomers, but at the expense of lower productivity compared to 2018 – given strong cost drivers around productivity for aerobic fermentation as documented previously [2], the higher productivity/lower titer case from 2018 was maintained for the “model compound” scenario. Key details for the lignin train as originally presented in the 2018 SOT are repeated below for context.

For the “base” lignin utilization case reflecting experimental work on integrated hydrolysate, actual black liquor and BCD product streams were fed to a lignin converting strain of *P. putida*. Experimental yields of muconic acid at 0.15 g/g total solubilized lignin and productivities of 0.06 g/L/hr were observed for both streams. Based on the mass balance in the SOT model this translates to an overall utilization of solubilized lignin of 16%. In other words, current bench scale work is achieving high solubilization of lignin but producing lignin species

(monomers/dimers/trimers/etc.) that are not consumed in high fractions by the current strain and at a slow rate. This incomplete consumption and slow kinetics are actively under investigation to determine the presence and impact of inhibitory species as well as improve the deconstruction process to target more convertible species. As noted earlier, carbohydrates and other oxygenated organic species (e.g., extractives) are degraded to shorter acids prior to entering the lignin fermentation. In the current model, these degradation products remain unconsumed, eventually reaching the wastewater treatment area where they are degraded. Muconic acid produced in the fermentation is recovered and upgraded to adipic acid as per the target parameters in the 2018 design case [2].

To understand the impacts of the strain engineering efforts surrounding the lignin fermentation a second “high performance” conceptual lignin case was explored based on data with model compounds. This case maintains similar assumptions and parameters for the BCD and black liquor composition but differs through the muconic acid fermentation. In 2018, bench scale data using mock lignin compounds (p-Coumaric acid) showed improved productivities of 0.53 g/L/hr under more controlled and optimal conditions, with a muconic acid titer of 27 g/L. In 2019, a higher titer was achieved at 48 g/L, but at a lower productivity of 0.40 g/L/hr. As noted above, given a strong cost driver around productivity at such levels (until roughly 1.0 g/L/hr, at which point the cost sensitivity begins to reduce) [2], along with no other process changes otherwise i.e. regarding yield to convertible species, the 2018 basis was maintained to minimize MFSP for this model lignin compound scenario. Accordingly, this higher productivity was used to benchmark the impact of a more optimized hypothetical fermentation. Importantly the overall muconic acid yield for this case was held constant at 0.15g/g as the conditioning and clarification steps are unchanged and the expected utilization of soluble lignin species would be identical with only 16% of *total available* lignin utilized by the strain. As improved analytical details become available on the complex BCD and black liquor, the added precision surrounding which specific species are inhibitory, utilized, and underutilized is expected to point toward improved strategies for tuning upstream conditioning and lignin deconstruction.

Results

TEA Results

Based on the details provided above for current experimental baselines across the integrated processes, the 2019 SOT benchmark for the **BDO pathway (“burn lignin” scenario)** is estimated at an overall MFSP of **\$7.79/GGE total or \$5.67/GGE for conversion-related costs (2016 dollars)** excluding feedstock allocations, with feedstock cost set at \$81.37/dry ton, associated with a 5% ash-equivalent biomass composition as described previously. This corresponds to an overall fuel yield of 38.5 GGE/ton biomass (22.1% carbon yield to fuels from starting biomass). Key process/TEA results are shown in Table 2, with further cost details provided in Appendix A. This result represents roughly \$1.23/GGE (14%) lower MFSP relative to last year’s 2018 SOT case for the BDO pathway (\$9.02/GGE in 2016-dollars) when viewed on comparable footing, i.e., based on burning lignin in the 2019 case and updating the underlying model framework consistently for the 2018 case. This cost reduction is driven primarily by considerably improved yields in enzymatic hydrolysis to sugars (mainly 8% increase in glucan to glucose maintaining the same 12 mg/g total enzyme loading as in the 2018 SOT), along with improved BDO fermentation yields (roughly 2% higher overall process yield to BDO) and productivities (30% increase), and finally improved aqueous BDO upgrading conversion to butene (11% increase). The above yield metrics supported an improvement in overall fuel yield from 32.3 to 38.5 GGE/ton, which is particularly notable given the more recalcitrant Lot 14 feedstock utilized this year and initial convertibility challenges this incurred as discussed above.

Similar to the findings in last year’s 2018 SOT, the 2019 SOT yield and MFSP results are challenged by relatively high losses of carbohydrates (primarily xylan and arabinan) into the DMR liquor phase, at least relative to what may be possible with more mild deacetylation as had been utilized previously in DDA pretreatment; however, the conditions employed here for DMR are currently seen to provide the best pretreatment/hydrolysis efficacy and overall MFSP optimization when DMR is required, as is the case in moving towards lignin coproduct upgrading (which is also ultimately targeted to make use of the solubilized carbohydrates in the future). For the BDO pathway SOT scenarios reflecting **lignin utilization**, the **MFSP is estimated at \$10.80/GGE for the “base case” fermentation performance** on actual hydrolysate, which would hypothetically reduce to **\$9.72/GGE for the “high” performance basis** on model lignin monomers (primarily higher productivity, while keeping muconic/adipic acid yields fixed). These results are associated with roughly 85% solubilization of residual solid lignin recovered from downstream processing, 16% of which is convertible across lignin fermentation at a muconic acid process yield of 0.16 g/g total soluble lignin. Given the low fraction of convertible species in the solubilized lignin material, the overall adipic acid process yields are roughly 15% of their final 2030 targets (2.3% vs 14.4% overall carbon yield to fuels from starting biomass respectively), which combined with 50-94% lower fermentation productivities (and accordingly higher fermentation/ processing costs), translates to a *net cost penalty* when lignin coproducts are included reflecting higher costs to produce the coproduct than the revenue it generates. To date, lignin conversion performance remains the same as was initially demonstrated in the 2018 SOT, which is not yet at a break-even point compared to lignin combustion; accordingly, significant room for improvement remains moving forward as the key factor in ultimately enabling future MFSP targets by 2030.

Utilizing the inputs from experimental work for the **carboxylic acids pathway (“burn lignin” scenario)**, an overall MFSP of **\$8.20/GGE total or \$5.90/GGE for conversion-related costs (2016-dollars)** excluding feedstock allocations is estimated for the 2019 SOT. This corresponds to an overall fuel yield of 35.3 GGE/ton biomass (20.6% carbon yield to fuels from starting biomass). Key process/TEA results are again shown in Table 2, with further cost details provided in Appendix A. Compared to last year’s 2018 SOT basis at \$10.40/GGE for an updated back-cast SOT model utilizing a consistent modeling framework, this represents a substantial improvement of \$2.20/GGE (21%) driven in large part by improved sugar yields across enzymatic hydrolysis as noted above for the BDO case as well as improvements across several fermentation parameters. While product yields from glucose improved by 6% (95%) when compared to 2018 numbers (90%), yields from xylose improved by nearly 19%, from 77% to 95% conversion of xylose to products, exceeding 2030 targets (which had originally been set before a good understanding was established for the xylose utilization ability of *C. tyrobutyricum*). Moreover, 2019 SOT yields also improved due to a continued improvement in the ratio of butyric : acetic acid (roughly 50:1, versus 2018 at 10:1 and 2017 at 3:1), given that acetic acid is ultimately lost in high amounts through both lower pertraction recoveries as well as higher losses to aqueous separations through catalytic upgrading. For the alternative acids pathway SOT scenarios reflecting **lignin utilization**, the **MFSP is estimated at \$11.47/GGE for the “base case” fermentation performance** on actual hydrolysate, which would hypothetically reduce to **\$10.29/GGE for the “high” performance basis** on model lignin monomers, based on maintaining the same lignin deconstruction and conversion parameters as noted above for the BDO case. Compared with the 2018 SOT results for the “base case” and “high” performance lignin coproduct scenarios, this leads to reductions of \$3.19/GGE and \$2.87/GGE, respectively, although due exclusively to fuel train improvements given no change in the lignin train performance as noted above. As discussed above, a 95% conversion of xylose to acids was set here, as asserted to be realistic in an optimized sugar feeding/acids pertraction operation. Under the experimentally measured value of 70% overall xylose utilization (67% to acids) as observed at the end of the fermentation run, this would translate to an MFSP of **\$8.97/GGE, \$12.60/GGE, and \$11.30/GGE** for the burn, convert (base), and convert (high) lignin scenarios, respectively (roughly 9%-10% higher MFSP), at a fuel yield of **32.2 GGE/ton** (9% lower yield).

Table 2(a). BDO Pathway: Technical Summary Table for 2019 SOT Benchmark, 2017-2018 Back-Cast SOT, and Future 2030 Targets [2]

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2019 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin (Base)^a	Convert Lignin (High)^a	Burn Lignin	Convert Lignin (Base)^a	Convert Lignin (High)^a	Convert Lignin
Projected Minimum Fuel Selling Price	\$/GGE	\$10.08	\$9.02	\$12.81	\$11.54	\$7.79	\$10.80	\$9.72	\$2.47
Feedstock Contribution	\$/GGE	\$2.67	\$2.59	\$2.59	\$2.59	\$2.11	\$2.11	\$2.11	\$1.65
Conversion Contribution	\$/GGE	\$7.41	\$6.43	\$10.22	\$8.95	\$5.67	\$8.69	\$7.61	\$0.82
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	31.4	32.3	32.3	32.3	38.5	38.5	38.5	43.2
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	40	40	0	42	42	266
Feedstock									
Feedstock Cost ^b	\$/dry U.S. ton	\$83.90	\$83.67	\$83.67	\$83.67	\$81.37	\$81.37	\$81.37	\$71.26
Pretreatment									
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids Loading	wt%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	92	90	90	90	92
Reactor Mode	Batch vs Counter-Current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter-Current
Total Caustic (NaOH) Loading	mg/g dry biomass	70	70	70	70	80	80	80	70
Net solubilized lignin to liquor	%	47%	47%	47%	47%	50%	50%	50%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	2%	2%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	17%	16%	16%	16%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	46%	46%	30%
Enzymatic Hydrolysis									
Hydrolysis Configuration	Batch vs CEH	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch
Total Solids Loading to Hydrolysis	wt%	20%	20%	20%	20%	20%	20%	20%	25%
Enzymatic Hydrolysis Batch Time	days	5	5	5	5	5	5	5	5
Hydrolysis Glucan to Glucose	%	78%	78%	78%	78%	84%	84%	84%	90%
Hydrolysis Xylan to Xylose	%	85%	85%	85%	85%	82%	82%	82%	90%
Sugar Loss (into solid stream after EH separation)	%	5%	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)	NA (whole slurry)
Cellulase Enzyme Production									
Enzyme Loading	mg/g cellulose	12	12	12	12	12	12	12	10
Fermentation, Catalytic Conversion, and Upgrading to Fuels									
Bioconversion Volumetric Productivity	g/L/hour	1.7	1.1	1.1	1.1	1.43	1.43	1.43	2.6
Glucose to Product [total glucose utilization] ^c	%	86% [100%]	95% [100%]	95% [100%]	95% [100%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	95% [98%]
Xylose to Product [total xylose utilization] ^c	%	89% [97%]	90% [92%]	90% [92%]	90% [92%]	89% [92%]	89% [92%]	89% [92%]	90% [92%]

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2019 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Convert Lignin
Arabinose to Product [total arabinose utilization] ^c	%	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	85% [89%]
Bioconversion Metabolic Yield (Process Yield)	g/g sugars	0.44 (0.42)	0.48 (0.46)	0.48 (0.46)	0.48 (0.46)	0.49 (0.46)	0.49 (0.46)	0.49 (0.46)	0.47 (0.45)
Fermentation intermediate product recovery	wt%	99.70%	96.80%	96.80%	96.80%	97.65%	97.65%	97.65%	96.40%
Aqueous BDO Upgrading: WHSV	hr ⁻¹	1	1	1	1	1	1	1	2
Aqueous BDO Upgrading: Per-pass conversion	wt% to desired products	89%	90%	90%	90%	100%	100%	100%	100%
Oligomerization: WHSV	hr ⁻¹	1	1	1	1	1	1	1	1
Oligomerization: Per-pass conversion	wt% to desired products	100%	100%	100%	100%	100%	100%	100%	100%
Hydrotreating: WHSV	hr ⁻¹	5	5	5	5	5	5	5	5
Hydrotreating: Per-pass conversion	wt% to desired products	100%	100%	100%	100%	100%	100%	100%	100%
Lignin Processing to Coproduct									
Solid Deconstruction to Soluble Lignin	wt% BCD lignin feed	-	-	85% ^e	85% ^e	-	85% ^e	85% ^e	53%
Convertible Components in Soluble Lignin	wt% of total soluble lignin (APL +BCD)	-	-	16%	16%	-	16%	16%	98%
Muconic Acid Process Yield from Lignin	g/g soluble lignin	-	-	0.15	0.15	-	0.16	0.16	1.59
Muconic Acid Metabolic Yield from Lignin	g/g lignin consumed	-	-	0.93	0.93	-	0.93	0.93	0.93
Overall Carbon Upgrading Efficiency to Coproduct ^d	mol%	-	-	3.80%	3.80%	-	3.80%	3.80%	27.80%
Muconic Acid Productivity	g/L/hr	-	-	0.06	0.53	-	0.06	0.53	1
Adipic Acid Production	MMlb/yr	-	-	29	29	-	30	30	193

^a 2018/2019 lignin conversion "base" case from actual black liquor/BCD hydrolysate; "high" case = highest productivity observed to date based on model lignin monomers

^b Feedstock costs shown here based on a 5% "ash equivalent" and 20% "moisture equivalent" basis for all years considered, consistent with values provided by Idaho National Laboratory for total feedstock costs and associated ash and moisture "dockage" costs for each year.

^c First number represents sugar conversion to desired product (BDO/acids); values in parentheses indicate total sugar utilization (including biomass organism propagation).

^d Includes fermentation of all convertible components, product recovery (crystallization) efficiencies, and hydrogenation yields to adipic acid (overall convertible C to adipic acid)

^e SOT assumes only post-EH lignin solids are routed through BCD, target cases route both lignin solids and DMR liquor through BCD. "Solubilized" lignin remains low in convertible components for SOT cases relative to future targets, translating to lower overall carbon efficiency to adipic acid coproduct.

Table 2(b). Acids Pathway: Technical Summary Table for 2019 SOT Benchmark, 2017-2018 Back-Cast SOT, and Future 2030 Targets [2]

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2019 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Convert Lignin
Projected Minimum Fuel Selling Price	\$/GGE	\$11.05	\$10.40	\$14.66	\$13.16	\$8.20	\$11.47	\$10.29	\$2.49
Feedstock Contribution	\$/GGE	\$3.19	\$2.99	\$2.99	\$2.99	\$2.30	\$2.30	\$2.30	\$1.59
Conversion Contribution	\$/GGE	\$7.86	\$7.41	\$11.67	\$10.17	\$5.90	\$9.17	\$7.98	\$0.90
Total Gasoline Equivalent Yield	GGE/dry U.S. ton	26.3	28	28	28	35.3	35.3	35.3	44.8
Adipic Acid Coproduct Yield	lb/dry ton biomass	0	0	41	41	0	42	42	259
Feedstock									
Feedstock Cost ^b	\$/dry U.S. ton	\$83.90	\$83.67	\$83.67	\$83.67	\$81.37	\$81.37	\$81.37	\$71.26
Pretreatment									
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids Loading	wt%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	92	90	90	90	92
Reactor Mode	Batch vs. Counter-Current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter-Current
Total Caustic (NaOH) Loading	mg/g dry biomass	70	70	70	70	80	80	80	70
Net solubilized lignin to liquor	%	47%	47%	47%	47%	50%	50%	50%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	2%	2%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	17%	16%	16%	16%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	46%	46%	30%
Enzymatic Hydrolysis									
Hydrolysis Configuration	Batch vs. CEH	Batch	Batch	Batch	Batch	Batch	Batch	Batch	CEH
Total Solids Loading to Hydrolysis	wt%	20%	20%	20%	20%	20%	20%	20%	7.60%
Enzymatic Hydrolysis Batch Time	days	5	5	5	5	5	5	5	Continuous
Hydrolysis Glucan to Glucose	%	78%	78%	78%	78%	84%	84%	84%	96%
Hydrolysis Xylan to Xylose	%	85%	85%	85%	85%	82%	82%	82%	99%
Sugar Loss (into solid stream after EH separation)	%	5%	5%	5%	5%	5%	5%	5%	1%
Cellulase Enzyme Production									
Enzyme Loading	mg/g cellulose	12	12	12	12	12	12	12	10
Fermentation, Catalytic Conversion, and Upgrading to Fuels									
Bioconversion Volumetric Productivity	g/L/hour	1.1	0.3	0.3	0.3	0.62	0.62	0.62	2
Glucose to Product [total glucose utilization] ^c	%	86% [100%]	90% [95%]	90% [95%]	90% [95%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [100%]
Xylose to Product [total xylose utilization] ^c	%	82% [100%]	77% [90%]	77% [90%]	77% [90%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	85% [100%]

	Units	2017 SOT	2018 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2019 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Burn Lignin	Convert Lignin (Base) ^a	Convert Lignin (High) ^a	Convert Lignin
Arabinose to Product [total arabinose utilization] ^c	%	82% [100%]	32% [38%]	32% [38%]	32% [38%]	20% [29.0%]	20% [29.0%]	20% [29.0%]	85% [87%]
Bioconversion Metabolic Yield (Process Yield)	g/g sugars	0.44 (0.44)	0.45 (0.41)	0.45 (0.41)	0.45 (0.41)	0.46 (0.44)	0.46 (0.44)	0.46 (0.44)	0.45 (0.43)
Fermentation intermediate product recovery	wt%	60% (C2), 95% (C4)	60% (C2), 95% (C4)	60% (C2), 95% (C4)	60% (C2), 95% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	100% (C4)
Ketonization: WHSV	hr ⁻¹	6	4	4	4	4	4	4	6
Ketonization: Per-pass conversion	wt% to desired products	100%	100%	100%	100%	100%	100%	100%	100%
Condensation: WHSV	hr ⁻¹	0.5	10 hr residence time	10 hr residence time	10 hr residence time	10 hr residence time	10 hr residence time	10 hr residence time	15 hr batch
Condensation: Overall conversion	wt% to desired products	81%	92%	92%	92%	92%	92%	92%	60% pp
Hydrotreating: WHSV	hr ⁻¹	3	4.7	4.7	4.7	4.7	4.7	4.7	3
Hydrotreating: Per-pass conversion	wt% to desired products	100%	100%	100%	100%	100%	100%	100%	100%
Lignin Processing to Coproduct									
Solid Deconstruction to Soluble Lignin	wt% BCD lignin feed	-	-	85% ^e	85% ^e	-	85% ^e	85% ^e	53%
Convertible Components in Soluble Lignin	wt% of total soluble lignin (APL +BCD)	-	-	16%	16%	-	16%	16%	98%
Muconic Acid Process Yield from Lignin	g/g soluble lignin	-	-	0.15	0.15	-	0.16	0.16	1.59
Muconic Acid Metabolic Yield from Lignin	g/g lignin consumed	-	-	0.93	0.93	-	0.93	0.93	0.93
Overall Carbon Upgrading Efficiency to Coproduct ^d	mol%	-	-	4.00%	4.00%	-	4.00%	4.00%	30.10%
Muconic Acid Productivity	g/L/hr	-	-	0.06	0.53	-	0.06	0.53	1
Adipic Acid Production	MMlb/yr	-	-	30	30	-	31	31	187

^a 2018/2019 lignin conversion “base” case from actual black liquor/BCD hydrolysate; “high” case = highest productivity observed to date based on model lignin monomers

^b Feedstock costs shown here based on a 5% “ash equivalent” and 20% “moisture equivalent” basis for all years considered, consistent with values provided by Idaho National Laboratory for total feedstock costs and associated ash and moisture “dockage” costs for each year.

^c First number represents sugar conversion to desired product (BDO/acids); values in parentheses indicate total sugar utilization (including biomass organism propagation).

^d Includes fermentation of all convertible components, product recovery (crystallization) efficiencies, and hydrogenation yields to adipic acid (overall convertible C to adipic acid)

^e SOT assumes only post-EH lignin solids are routed through BCD, target cases route both lignin solids and DMR liquor through BCD. “Solubilized” lignin remains low in convertible components for SOT cases relative to future targets, translating to lower overall carbon efficiency to adipic acid coproduct.

Table 2 and Figure 2 also show the detailed comparisons between the 2019 SOT scenarios, the 2018/2017 back-cast SOTs after updating for consistent model framework, and the future design case targets moving forward to achieving <\$2.50/GGE by 2030. Moving forward to those future out-year projections, room for further improvement exists to varying degrees across all major processing steps. Namely, DMR pretreatment must move towards reducing water consumption, increasing black liquor concentration, and reducing carbohydrate (xylan/arabinan) losses by incorporating the continuous counter-current alkaline extraction design described in the 2018 design report. Enzymatic hydrolysis must continue moving towards higher sugar yields (primarily 90% targets vs 82-84% SOT for glucan and xylan conversion respectively) at further reduced enzyme loadings (10 vs. 12 mg total enzyme/g cellulose). Early experimental indications suggest promising performance moving forward, but solving these issues requires not only more fundamental understanding of biomass recalcitrance but also continuous collaborations and efforts between national lab and enzyme companies to develop and improve enzyme packages. In the acids case, the CEH concept must be further developed and eventually integrated into the process to demonstrate efficacy and the ability to at least match, or more ideally exceed, performance for standard batch EH with respect to sugar yields and enzyme loading.

Sugar fermentation and catalytic upgrading performance must also be improved beyond 2019 SOT benchmarks. In the BDO pathway, fermentation yields have nearly achieved final 2030 goals already (on whole slurry hydrolysate), with exception of arabinose utilization which must be engineered into the organism, while also nearly doubling the fermentation productivity. The larger area of future work remains in demonstrating fully anaerobic production of BDO rather than minimal oxygen intake via fermentor air overlay (or otherwise better understanding microaerophilic bioreactor design in the TEA models). BDO upgrading yields also have further room for improvement, primarily with respect to the aqueous BDO upgrading step, requiring a doubling in catalyst WHSV and catalyst lifetime. In the acids pathway, fermentation yields are similarly high for glucose and xylose (meeting or exceeding 2030 targets) but also require more improvement on arabinose utilization, while continuing to optimize operational fed-batch feeding rates to demonstrate the capability to continuously maintain high glucose and xylose conversions, and also improving productivity by roughly a factor of three (2.0 g/L-hr targets vs 0.6 g/L-hr SOT basis). Pertractive recovery of acids, while now based on a real hydrolysate fermentation substrate, must also be further optimized to demonstrate the ability to recycle solvents without impacting organism performance over extended time periods. Alternative approaches to pertraction are currently under investigation, for example based on electro dialysis to recycle the salts as being investigated by ANL (with NREL TEA support) under the Separations Consortium. Efforts are also ongoing under the ChemCatBio CUBI project to further optimize acids upgrading operations, with the current set of parameters projecting further improvements in ketonization WHSV and further optimized condensation parameters.

Finally, the largest single area for more substantial improvements is in the lignin-to-coproducts train. As noted above and consistent with the 2018 SOT, despite the high value of the adipic acid coproduct, the current experimental benchmark data translates to a higher cost to produce the adipic acid than the coproduct revenues it generates, driven most strongly by low bioconversion productivity to muconic acid (translating to large fermentor volumes and costs for this aerobic fermentation step), but also significantly by low deconstruction to soluble/convertible lignin components (as well as no credit yet assumed for productive conversion of either carbohydrates or biomass extractives in black liquor to muconic acid). Relative to 2018/19 SOT benchmark

levels, the lignin train must improve by 2030 to achieve a 17-fold improvement in productivity (from 0.06 up to 1.0 g/L-hr, although productivity on model lignin monomer compounds is considerably higher at 0.5 g/L-hr) and 10-fold improvement in overall lignin conversion (from 0.16 to 1.6 g/g soluble lignin process yields, translating to overall carbon yield improvement from 4% to 30% from convertible carbon through adipic acid), in order to improve overall adipic acid outputs from 31 to roughly 190 MM lb/yr in the modeled biorefinery. Given that this undoubtedly represents a more substantial required degree of improvement than most other process areas, as well as the fact that performance has not yet been improved for the lignin coproduct train in 2019 beyond initial levels demonstrated in 2018, this generally represents the largest-risk area of the integrated process in ultimately achieving future MFSP goals. As such, in 2020 the Biochemical Analysis project is planning to continue a primary focus around evaluating potential alternative “contingency strategies” that also may enable MFSP reductions through other processing approaches (based on NREL experimental efforts being undertaken in such areas).

Figure 2 provides a waterfall plot of MFSP cost breakdowns by process area, reflecting all cases listed in Table 2.

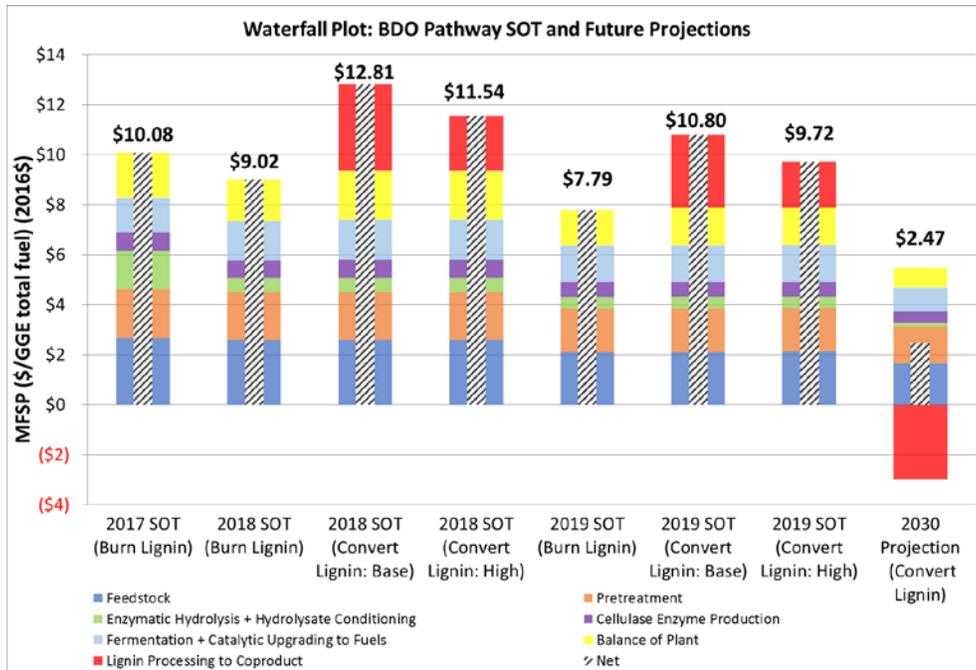


Figure 2(a). Tracking SOT progression from 2017-2019, compared to out-year 2030 projection (BDO pathway)

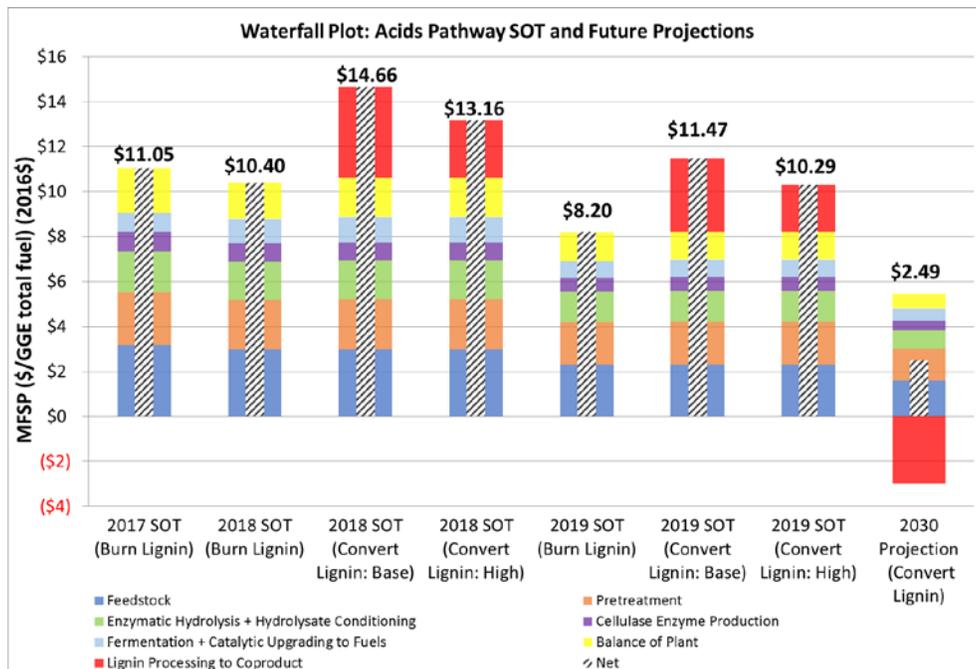


Figure 2(b). Tracking SOT progression from 2017-2019, compared to out-year 2030 projection (acids pathway)

Sustainability Metric Indicators

In addition to the TEA results noted above, here we also report on associated sustainability “indicators” attributed to the SOT conversion model scenarios. In keeping with recent Bioenergy Technologies Office (BETO) guidance for all formal LCA sustainability metrics to be handled by ANL to ensure no inconsistencies in such metrics versus NREL-calculated values (i.e., using GREET versus SimaPro), we avoid reporting on LCA parameters such as greenhouse gas emissions or fossil energy consumption in this report (but will provide the input/output inventories to partners at ANL). Instead, Table 3 summarizes key sustainability indicators as may be taken directly from the Aspen Plus process models for all cases presented in Table 2. Namely, this includes mass and carbon yield to fuels, carbon yield to coproducts, facility power and natural gas demands, and water consumption for the conversion process. The process input/output inventories to be furnished to ANL for subsequent LCA supply chain sustainability analysis (SCSA) are summarized in Appendix B.

Both pathways reflect an increase in mass/carbon yield to fuels for the 2019 SOT cases relative to 2018 attributed to improved enzymatic hydrolysis glucose yields and fermentation yields (more substantially improved in the acids case), as well as catalytic upgrading yields in the BDO case. Both pathways also require a net power import in all cases evaluated due to power demands throughout the facility (driven by mechanical refining pretreatment, MVR sugar evaporation where relevant, and aerobic lignin bioconversion power demands) as well as heat demands diverting steam away from the steam turbine generators. Both cases showed slight increases in power demand relative to 2018 in the case of burning lignin, due in part to upstream changes in solubilization, carbohydrate hydrolysis, and conversion leading to less unconverted biomass available to be burned for heat and power. In the BDO case compared to 2018, there is a slight decrease in the amount of natural gas imported to meet heat demands in the “convert lignin” scenarios due in part to a reduced heat demand enabled by improvements to the BDO upgrading and purification areas of the plant. Water consumption also decreased for all cases in 2019 due to reduced cooling water demands and improvements to the product selectivity and recovery, requiring less water in product scrubbers for the acids cases.

Table 3. Sustainability Indicators for 2017-2019 SOT and Future Projection Scenario

	2017 SOT (Burn Lignin)	2018 SOT (Burn Lignin)	2018 SOT Convert Lignin (Base)	2018 SOT Convert Lignin (High)	2019 SOT (Burn Lignin)	2019 SOT Convert Lignin (Base)	2019 SOT Convert Lignin (High)	2030 Projection (Convert Lignin)
BDO Pathway								
Fuel Yield by Weight of Biomass (wt% of dry biomass)	9.6%	9.9%	9.9%	9.9%	11.7%	11.7%	11.7%	13.2%
Carbon Efficiency to Fuels (% feedstock C)	18.2%	18.7%	18.7%	18.7%	22.1%	22.1%	22.1%	25.0%
Carbon Efficiency to Lignin Coproduct (% feedstock C)	NA	NA	2.3%	2.3%	NA	2.3%	2.3%	14.8%
Net Electricity Import (kWh/GGE)	12.3	5.1	14	14	5.7	12.5	12.6	10.5
Net Natural Gas Import (Btu/GGE [LHV])	0	0	75,284	76,789	0	69,928	69,928	14,596
Water Consumption (gal water/GGE)	23.4	13.9	11.3	11.5	10.9	9.2	9.2	8.9
Acids Pathway								
Fuel Yield by Weight of Biomass (wt% of dry biomass)	8.1%	8.6%	8.6%	8.6%	10.8%	10.8%	10.8%	13.8%
Carbon Efficiency to Fuels (% feedstock C)	15.5%	16.3%	16.3%	16.3%	20.6%	20.6%	20.6%	26.2%
Carbon Efficiency to Lignin Coproduct (% feedstock C)	NA	NA	2.3%	2.3%	NA	2.3%	2.3%	14.4%
Net Electricity Import (kWh/GGE)	5.8	1.3	21.5	21.6	2.8	17.4	17.6	10.7
Net Natural Gas Import (Btu/GGE [LHV])	0	15,790	15,790	15,790	11,803	11,803	11,803	9,055
Water Consumption (gal water/GGE)	30.7	36.03	26	26.1	27.7	20	20	13.5

Concluding Remarks

The work presented here provides a re-benchmarking of NREL's Biochemical Platform efforts in moving towards future design case goals. Based on data availability for 2019 experimental work on integrated hydrolysate processing, the 2019 SOT considers two bioconversion pathways for hydrocarbon fuel production, namely BDO and carboxylic acids. Biomass deconstruction efforts presently reflect 84% glucan conversion, 82% xylan conversion, and 55% arabinan conversion to monomeric sugars through saccharification at 12 mg/g enzyme loading, based on new DMR pretreatment and batch enzymatic hydrolysis performance data observed in 2019. One confounding factor in the 2019 SOT experimental work was a switch to a new, more recalcitrant source of corn stover feedstock (INL Lot 14), which required more severe DMR conditions than historically applied in prior SOTs; however, after increasing DMR severity (NaOH loading), overall yields were shown to improve over prior SOT levels (following initial challenges imparted on some downstream operations such as BDO fermentation, which were subsequently overcome). Bioconversion and catalytic upgrading performance for both fuel pathways was quite favorable, utilizing over 95% of glucose and 89% of xylose sugars at fermentation process yields approaching or exceeding final design case targets (albeit at lower productivities relative to final targets), and catalytic conversions of 100% to fuel products across all steps that were experimentally demonstrated (albeit at lower space velocities in some steps than final targets). **The resulting 2019 SOT benchmark MFSPs are estimated to be \$7.79/GGE and \$8.20/GGE (\$5.67/GGE and \$5.90/GGE conversion-only costs excluding feedstock contributions at \$81/ton) in 2016-dollars based on combustion of all lignin and residual solids, for the BDO and acids pathways respectively.** Relative to a 2018 back-cast SOT basis, this translates to an improvement of \$1.23/GGE (14%) and \$2.20/GGE (21%) in overall MFSPs for the two respective pathways.

Alternative SOT scenarios were also evaluated inclusive of lignin conversion to coproducts, with 2019 SOT MFSP estimates of **\$10.80/GGE and \$11.47/GGE for “base case” lignin conversion** performance on biomass hydrolysate (BDO and acids pathways respectively); this would hypothetically reduce to **\$9.72/GGE and \$10.29/GGE for “high” lignin conversion** performance as observed for model lignin monomers. These results indicate that the lignin-to-coproduct train is not yet economically profitable relative to burning the lignin, given higher costs for producing the adipic acid coproduct than the amount of coproduct revenue generated (attributed in turn to low lignin deconstruction/conversion yields and fermentation productivities observed to date). Performance parameters for the lignin coproduct train were generally not shown to be improved in 2019 beyond initial demonstration levels in the prior 2018 SOT. As an alternative sensitivity scenario for the acids pathway, when reflecting experimentally measured values for xylose fermentation to acids (67% to product) in place of the performance asserted to be realistic for an optimized sugar feeding/pertraction operational approach (95% to product), the acids pathway MFSPs would increase by roughly 9% (**\$8.97/GGE, \$12.60/GGE, and \$11.30/GGE for burn, convert [base], and convert [high] lignin cases, respectively**), with a similar 9% reduction in fuel yield.

Analysis of sustainability metric indicators from the Aspen SOT conversion models demonstrates BDO fuel yields of 11.7% by weight or 22.1% by carbon retention relative to biomass feedstock, along with 2.3% carbon yields to adipic acid coproduct in the “convert lignin” scenarios. Fuel yields are slightly lower for the acids case at 10.8% by weight or 20.6%

by carbon utilization, with the same 2.3% carbon yield basis to adipic acid. Net power imports are calculated as 5.7 kWh/GGE for the BDO case or 2.8 kWh/GGE for the acids case in the “burn lignin” scenario, increasing to 12.5 and 17.4 respectively in the “convert lignin” scenario (due to substantial power demands for aerobic lignin bioconversion at low fermentation productivities). Approximately 70,000 Btu/GGE of supplemental natural gas is required for the 2019 SOT BDO cases including lignin conversion but none is required for the “burn lignin” scenario, while for the acids case, roughly 12,000 Btu/GGE of natural gas is required in all 2019 SOT cases as a means to provide necessary utility trim heating for catalytic upgrading process temperature demands. Finally, water consumption is estimated at 10.9 gal/GGE for the BDO “burn lignin” case, and roughly 9.2 gal/GGE for the BDO “convert lignin” case. Water consumption is higher at 27.7 in the acids “burn lignin” case, reducing to 20.0 in the “convert lignin” case, driven in part by still requiring the hydrolysate solid/liquid separation and water wash step.

Moving forward, further room for improvement exists to reduce costs to 2030 goals. Namely, deconstruction must further improve sugar yields at lower enzyme loadings while also better optimizing DMR costs by way of increasing DMR liquor concentrations and reducing carbohydrate losses into the soluble liquor fraction (e.g. through continuous counter-current alkaline extraction rather than batch deacetylation), also with significant room for potential improvement moving forward if sodium hydroxide usage could either be reduced or recovered and recycled. Deconstruction improvements also include integrating and demonstrating continuous enzymatic hydrolysis into the process as a means to further reduce costs in the acids pathway. Additionally, fuel-train fermentation and catalytic upgrading yields, as well as recoveries of intermediate products, must also be further improved, in line with final design case targets (although many associated parameters are beginning to approach or in some cases exceed final targets already). A key parameter for further R&D focus and demonstration in the acids pathway will be low-cost recovery of the intermediate acids utilizing continuous pertraction at high recovery efficiencies, or alternative approaches to avoid significant fresh caustic/acid demands (including options being investigated under the Separations Consortium), or most ideally achieving low-pH fermentation without the need for any acids isolation operations. Finally, more significant improvements are required in the lignin coproduct train in order to first break even and ultimately lower MFSPs towards future 2030 targets. This primarily centers around increasing lignin deconstruction to convertible monomers, incorporating the capability to utilize other components such as carbohydrates and extractives, and improving bioconversion productivity to muconic acid (subsequently upgraded to adipic acid via mild hydrogenation).

References

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

- [1] AspenPlus, "Release 7.2, Aspen Technology Inc., Cambridge MA," 2007. Available: www.aspentech.com
- [2] Davis, R. E., N. J. Grundl, L. Tao, M. J. Bidy, E. C. D. Tan, G. T. Beckham, D. Humbird, D. N. Thompson, and M. S. Roni, "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," National Renewable Energy Lab (NREL), Golden, CO, 2018. Available: <https://www.nrel.gov/docs/fy19osti/71949.pdf>
- [3] Davis, R., M. Bidy, L. Tao, and N. Grundl, "FY18 Q2 Go/No Go – Pathway Down-Select for FY18 Design Report," NREL Milestone Report, 2018.
- [4] Davis, R., L. Tao, E. C. D. Tan, M. Bidy, G. T. Beckham, C. Scarlata, J. Jacobson, K. Cafferty, J. Ross, J. Lukas, D. Knorr, and P. Schoen, "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," National Renewable Energy Laboratory, Golden, CO, 2013. Available: <http://www.nrel.gov/docs/fy14osti/60223.pdf>
- [5] Chen, X., E. Kuhn, N. Nagle, R. Nelson, L. Tao, N. Crawford, and M. Tucker, "Recycling of Dilute Deacetylation Black Liquor to Enable Efficient Recovery and Reuse of Spent Chemicals and Biomass Pretreatment Waste," *Frontiers in Energy Research*, vol. 6, p. 51, 2018. Available: <https://doi.org/10.3389/fenrg.2018.00051>.
- [6] 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, "Process Design and Economics for Biocheical Conversion of Lignocellulosic Biomass to Ethanol," National Renewable Energy Laboratory (NREL), Golden, CO, 2011. Available: <http://www.nrel.gov/docs/fy11osti/47764.pdf>
- [7] Davis, R., L. Tao, C. Scarlata, E. C. D. Tan, J. Ross, J. Lukas, and D. Sexton, "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," National Renewable Energy Laboratory (NREL), Golden, CO, 2015. Available: <http://www.nrel.gov/docs/fy15osti/62498.pdf>
- [8] Chen, X., N. Nagle, L. Tao, and M. Tucker, "Show at least 5% improvement in sugar yields (>83% monomeric sugars at 12 mg protein/g glucan) over FY17 SOT yields by an ozone assisted DMR process over controls without ozone assisted chemistry. Metrics: Test at least 2 conditions of ozone pretreatment at 2 deacetylation severities, 2 refining energy consumptions and 2 enzyme loadings. (Low-Temperature Advanced Deconstruction FY19Q3)," NREL milestone report, 2019.
- [9] Davis, R., M. Bidy, L. Tao, N. Grundl, G. Beckham, N. Dowe, M. Himmel, and M. Zhang, "TEA Identification of Most Promising Options for 2022 Targets," NREL milestone report, 2016.

Appendix A. TEA Summary Sheets for 2019 SOT Benchmark Models (2016-dollars)

BDO Pathway (Burn Lignin)

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

DMR Pretreatment, Whole-slurry Enzymatic Hydrolysis & Anaerobic Bioconversion, Catalytic Upgrading, Lignin Combustion
All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$7.79 /GGE**

Contributions: Feedstock **\$2.12 /GGE**
Fuel Conversion **\$5.67 /GGE**
Coproduct Conversion **\$0.00 /GGE**

Fuel Production 27.9 MMGGE per year (at 68 °F)
Fuel Yield 38.5 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield 0 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield] 0.46 [0.5] kg BDO/kg Total Sugars (93% of theoretical)
Feedstock + Handling Cost \$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax) 10%
Equity Percent of Total Investment 40%

Capital Costs	
Area 200: Pretreatment	\$45,441,175
Area 300: Sugar Hydrolysis and Conditioning	\$20,228,637
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$69,555,969
Area 600: Wastewater	\$68,340,171
Area 700: Lignin	\$0
Area 800: Boiler	\$66,971,025
Area 900: Utilities & Storage	\$12,320,710

Total Installed Equipment Cost	\$296,230,206
Added Direct + Indirect Costs (% of TCI)	\$246,969,794 45%
Total Capital Investment (TCI)	\$543,200,000

Installed Equipment Cost/Annual GGE	\$10.64
Total Capital Investment/Annual GGE	\$19.50

Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.128

Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.8%
From Biomass (Fuel C / Biomass C)	22.1%
Adipic Acid Carbon Efficiency from Biomass	0.0%

Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	151,073
Current Fuel Production (U.S. ton/yr) ^b	84,840
Current Yield (Actual/Theoretical)	56.2%

^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)

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	211.6
Sulfuric Acid	0.0
Caustic	99.2
Glucose (enzyme production)	36.4
Hydrogen	36.0
Electricity (import)	37.3
Other Raw Materials	80.2
Catalysts	13.3
Waste Disposal	5.1
Na2SO4 Coproduct	-42.0
Adipic Acid coproduct (\$0.86/lb)	0.0
Fixed Costs	50.9
Capital Depreciation	61.7
Average Income Tax	19.1
Average Return on Investment	169.9
Total	778.8

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$0
Caustic	\$27,600,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$10,000,000
Electricity (import)	\$10,400,000
Other Raw Materials	\$22,300,000
Catalysts	\$3,700,000
Waste Disposal	\$1,400,000
Na2SO4 Coproduct	-\$11,700,000
Adipic Acid coproduct (\$0.86/lb)	\$0
Fixed Costs	\$14,200,000
Capital Depreciation	\$17,200,000
Average Income Tax	\$5,300,000
Average Return on Investment	\$47,300,000
Total	\$216,700,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	12.0
Net Electricity Import (kWh/GGE)	5.7
Plant Electricity Use (kWh/GGE)	14.3
Metabolic Yield (g/g substrate)	
Glucose to 2,3-BDO	0.477
Glucose to Biomass	0.016
Xylose to 2,3-BDO	0.487
Xylose to Biomass	0.017
Arabinos to 2,3-BDO	8.959
Arabinos to Biomass	0.328

BDO Pathway (Convert Lignin – “Base”)

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): **\$10.80 /GGE**

Contributions:	Feedstock	\$2.11 /GGE
	Fuel Conversion	\$5.76 /GGE
	Coproduct Conversion	\$2.93 /GGE

Fuel Production	27.9 MMGGE per year (at 68 °F)
Fuel Yield	38.5 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	42 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield]	0.46 [0.5] kg BDO/kg Total Sugars (93% of theoretical)
Feedstock + Handling Cost	\$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$45,441,175
Area 300: Sugar Hydrolysis and Conditioning	\$20,228,740
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$69,611,222
Area 600: Wastewater	\$60,569,673
Area 700: Lignin	\$273,236,358
Area 800: Boiler	\$52,149,330
Area 900: Utilities & Storage	\$14,530,207

Total Installed Equipment Cost	\$549,139,223
Added Direct + Indirect Costs (% of TCI)	\$499,260,777 48%
Total Capital Investment (TCI)	\$1,048,400,000

Installed Equipment Cost/Annual GGE	\$19.68
Total Capital Investment/Annual GGE	\$37.57

Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.128

Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.9%
From Biomass (Fuel C / Biomass C)	22.1%
Adipic Acid Carbon Efficiency from Biomass	2.3%

Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	151,073
Current Fuel Production (U.S. ton/yr) ^b	84,990
Current Yield (Actual/Theoretical)	56.3%

^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)

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	211.2
Sulfuric Acid	34.9
Caustic	147.4
Glucose (enzyme production)	36.3
Hydrogen	42.6
Electricity (import)	83.3
Other Raw Materials	96.8
Catalysts	14.0
Waste Disposal	5.2
Na2SO4 Coproduct	-71.2
Adipic Acid coproduct (\$0.86/lb)	-92.5
Fixed Costs	92.2
Capital Depreciation	119.0
Average Income Tax	35.9
Average Return on Investment	324.8
Total	1080.0

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$9,700,000
Caustic	\$41,100,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$11,900,000
Electricity (import)	\$23,200,000
Other Raw Materials	\$27,000,000
Catalysts	\$3,900,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$19,900,000
Adipic Acid coproduct (\$0.86/lb)	-\$25,800,000
Fixed Costs	\$25,700,000
Capital Depreciation	\$33,200,000
Average Income Tax	\$10,000,000
Average Return on Investment	\$90,600,000
Total	\$301,100,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	12.0
Net Electricity Import (kWh/GGE)	12.5
Plant Electricity Use (kWh/GGE)	15.7
Metabolic Yield (g/g substrate)	
Glucose to 2,3-BDO	0.477
Glucose to Biomass	0.016
Xylose to 2,3-BDO	0.487
Xylose to Biomass	0.017
Arabinos to 2,3-BDO	7.315
Arabinos to Biomass	0.268

BDO Pathway (Convert Lignin – “High”)

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): **\$9.72 /GGE**

Contributions:	Feedstock	\$2.11 /GGE
	Fuel Conversion	\$5.76 /GGE
	Coproduct Conversion	\$1.85 /GGE

Fuel Production	27.9 MMGGE per year (at 68 °F)
Fuel Yield	38.5 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	42 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield]	0.46 [0.5] kg BDO/kg Total Sugars (93% of theoretical)
Feedstock + Handling Cost	\$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$45,441,175
Area 300: Sugar Hydrolysis and Conditioning	\$20,228,740
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$69,611,222
Area 600: Wastewater	\$60,564,722
Area 700: Lignin	\$168,653,000
Area 800: Boiler	\$52,145,717
Area 900: Utilities & Storage	\$14,531,755

Total Installed Equipment Cost	\$444,548,848
Added Direct + Indirect Costs (% of TCI)	\$397,451,152 47%
Total Capital Investment (TCI)	\$842,000,000

Installed Equipment Cost/Annual GGE	\$15.93
Total Capital Investment/Annual GGE	\$30.18
Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.128

Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.9%
From Biomass (Fuel C / Biomass C)	22.1%
Adipic Acid Carbon Efficiency from Biomass	2.3%

Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	151,073
Current Fuel Production (U.S. ton/yr) ^b	84,990
Current Yield (Actual/Theoretical)	56.3%

^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)

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	211.2
Sulfuric Acid	34.9
Caustic	147.4
Glucose (enzyme production)	36.3
Hydrogen	42.6
Electricity (import)	84.1
Other Raw Materials	96.8
Catalysts	14.0
Waste Disposal	5.2
Na2SO4 Coproduct	-71.2
Adipic Acid coproduct (\$0.86/lb)	-92.5
Fixed Costs	76.1
Capital Depreciation	95.7
Average Income Tax	29.1
Average Return on Investment	262.3
Total	972.0

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$9,700,000
Caustic	\$41,100,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$11,900,000
Electricity (import)	\$23,500,000
Other Raw Materials	\$27,000,000
Catalysts	\$3,900,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$19,900,000
Adipic Acid coproduct (\$0.86/lb)	-\$25,800,000
Fixed Costs	\$21,200,000
Capital Depreciation	\$26,700,000
Average Income Tax	\$8,100,000
Average Return on Investment	\$73,200,000
Total	\$271,100,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	12.0
Net Electricity Import (kWh/GGE)	12.6
Plant Electricity Use (kWh/GGE)	15.8
Metabolic Yield (g/g substrate)	
Glucose to 2,3-BDO	0.477
Glucose to Biomass	0.016
Xylose to 2,3-BDO	0.487
Xylose to Biomass	0.017
Arabinos to 2,3-BDO	7.315
Arabinos to Biomass	0.268

Acids Pathway (Burn Lignin)

Biological Renewable Diesel Blendstock (RDB) via Butyric Acids: Process Engineering Analysis

DMR Pretreatment, Batch Enzymatic Hydrolysis, Hydrolysate Clarification, Anaerobic Bioconversion, Catalytic Upgrading, Lignin

Combustion

All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$8.20 /GGE**

Contributions:	Feedstock	\$2.30 /GGE
	Fuel Conversion	\$5.90 /GGE
	Coproduct Conversion	\$0.00 /GGE

Fuel Production	25.6 MMGGE per year (at 68 °F)
Fuel Yield	35.3 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	0 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.44 [0.49] kg Acid/kg Total Sugars (90% of theoretical)
Feedstock + Handling Cost	\$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$45,425,054
Area 300: Sugar Hydrolysis and Conditioning	\$75,139,452
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$46,299,175
Area 600: Wastewater	\$66,677,014
Area 700: Lignin	\$0
Area 800: Boiler	\$69,282,935
Area 900: Utilities & Storage	\$12,105,878

Total Installed Equipment Cost	\$328,302,026
Added Direct + Indirect Costs (% of TCI)	\$278,097,974 46%
Total Capital Investment (TCI)	\$606,400,000

Installed Equipment Cost/Annual GGE	\$12.84
Total Capital Investment/Annual GGE	\$23.71

Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.128

Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.5%
From Biomass (Fuel C / Biomass C)	20.6%
Adipic Acid Carbon Efficiency from Biomass	0.0%

Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr) ^b	78,472
Current Yield (Actual/Theoretical)	60.9%

^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)

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	230.5
Sulfuric Acid	0.0
Caustic	108.0
Glucose (enzyme production)	39.6
Hydrogen	0.0
Electricity (import)	17.1
Other Raw Materials	98.1
Catalysts	2.3
Waste Disposal	5.5
Na2SO4 Coproduct	-44.3
Adipic Acid coproduct (\$0.86/lb)	0.0
Fixed Costs	60.8
Capital Depreciation	75.1
Average Income Tax	23.0
Average Return on Investment	204.6
Total	820.4

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$0
Caustic	\$27,600,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$0
Electricity (import)	\$4,400,000
Other Raw Materials	\$25,100,000
Catalysts	\$600,000
Waste Disposal	\$1,400,000
Na2SO4 Coproduct	-\$11,300,000
Adipic Acid coproduct (\$0.86/lb)	\$0
Fixed Costs	\$15,500,000
Capital Depreciation	\$19,200,000
Average Income Tax	\$5,900,000
Average Return on Investment	\$52,300,000
Total	\$209,700,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	12.0
Net Electricity Import (kWh/GGE)	2.8
Plant Electricity Use (kWh/GGE)	17.4
Metabolic Yield (g/g substrate)	
Glucose to Butyric	0.465
Glucose to Biomass	0.021
Xylose to Butyric	0.465
Xylose to Biomass	0.021
Arabinos to Butyric	0.140
Arabinos to Biomass	0.021

Acids Pathway (Convert Lignin – “Base”)

Biological Renewable Diesel Blendstock (RDB) via Butyric Acids: Process Engineering Analysis

DMR Pretreatment, Batch Enzymatic Hydrolysis, Hydrolysate Clarification, Anaerobic Bioconversion, Catalytic Upgrading, Lignin Conversion to Coproducts

All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$11.47 /GGE**

Contributions:	Feedstock	\$2.30 /GGE
	Fuel Conversion	\$5.91 /GGE
	Coproduct Conversion	\$3.26 /GGE

Fuel Production	25.6 MMGGE per year (at 68 °F)
Fuel Yield	35.3 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	42 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.44 [0.49] kg Acid/kg Total Sugars (90% of theoretical)
Feedstock + Handling Cost	\$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$45,425,054
Area 300: Sugar Hydrolysis and Conditioning	\$75,139,452
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$46,284,117
Area 600: Wastewater	\$59,231,230
Area 700: Lignin	\$273,176,080
Area 800: Boiler	\$38,413,390
Area 900: Utilities & Storage	\$14,037,781
Total Installed Equipment Cost	\$565,079,623
Added Direct + Indirect Costs (% of TCI)	\$519,420,377 48%
Total Capital Investment (TCI)	\$1,084,500,000
Installed Equipment Cost/Annual GGE	\$22.09
Total Capital Investment/Annual GGE	\$42.40
Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.127
Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.5%
From Biomass (Fuel C / Biomass C)	20.6%
Adipic Acid Carbon Efficiency from Biomass	2.3%
Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr) ^b	78,473
Current Yield (Actual/Theoretical)	60.9%

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	230.5
Sulfuric Acid	40.6
Caustic	171.5
Glucose (enzyme production)	39.6
Hydrogen	0.0
Electricity (import)	117.1
Other Raw Materials	78.3
Catalysts	3.2
Waste Disposal	5.7
Na2SO4 Coproduct	-81.9
Adipic Acid coproduct (\$0.86/lb)	-102.3
Fixed Costs	105.3
Capital Depreciation	134.5
Average Income Tax	40.3
Average Return on Investment	365.0
Total	1147.4

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$10,400,000
Caustic	\$43,900,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$0
Electricity (import)	\$30,000,000
Other Raw Materials	\$20,000,000
Catalysts	\$800,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$20,900,000
Adipic Acid coproduct (\$0.86/lb)	-\$26,200,000
Fixed Costs	\$26,900,000
Capital Depreciation	\$34,400,000
Average Income Tax	\$10,300,000
Average Return on Investment	\$93,300,000
Total	\$293,400,000

^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)	12.0
Net Electricity Import (kWh/GGE)	17.4
Plant Electricity Use (kWh/GGE)	20.8
Metabolic Yield (g/g substrate)	
Glucose to Butyric	0.465
Glucose to Biomass	0.021
Xylose to Butyric	0.465
Xylose to Biomass	0.021
Arabinos to Butyric	0.140
Arabinos to Biomass	0.021

Acids Pathway (Convert Lignin – “High”)

Biological Renewable Diesel Blendstock (RDB) via Butyric Acids: Process Engineering Analysis

DMR Pretreatment, Batch Enzymatic Hydrolysis, Hydrolysate Clarification, Anaerobic Bioconversion, Catalytic Upgrading, Lignin Conversion to Coproducts

All Values in 2016\$

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis): **\$10.29 /GGE**

Contributions:	Feedstock	\$2.30 /GGE
	Fuel Conversion	\$5.92 /GGE
	Coproduct Conversion	\$2.06 /GGE

Fuel Production	25.6 MMGGE per year (at 68 °F)
Fuel Yield	35.3 GGE / dry U.S. ton feedstock
Adipic Acid Coproduct Yield	42 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.44 [0.49] kg Acid/kg Total Sugars (90% of theoretical)
Feedstock + Handling Cost	\$81.37 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	\$45,425,054
Area 300: Sugar Hydrolysis and Conditioning	\$75,139,452
Area 400: Enzyme Production	\$13,372,518
Area 500: Bioconversion and Upgrading	\$46,284,117
Area 600: Wastewater	\$59,226,398
Area 700: Lignin	\$167,773,242
Area 800: Boiler	\$38,424,494
Area 900: Utilities & Storage	\$14,039,230
Total Installed Equipment Cost	\$459,684,505
Added Direct + Indirect Costs (% of TCI)	\$416,715,495 48%
Total Capital Investment (TCI)	\$876,400,000
Installed Equipment Cost/Annual GGE	\$17.97
Total Capital Investment/Annual GGE	\$34.27
Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.128
Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	44.5%
From Biomass (Fuel C / Biomass C)	20.6%
Adipic Acid Carbon Efficiency from Biomass	2.3%
Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr) ^b	78,473
Current Yield (Actual/Theoretical)	60.9%

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	230.5
Sulfuric Acid	40.6
Caustic	171.5
Glucose (enzyme production)	39.6
Hydrogen	0.0
Electricity (import)	118.0
Other Raw Materials	78.3
Catalysts	3.2
Waste Disposal	5.7
Na2SO4 Coproduct	-81.9
Adipic Acid coproduct (\$0.86/lb)	-102.3
Fixed Costs	87.5
Capital Depreciation	108.7
Average Income Tax	32.8
Average Return on Investment	296.4
Total	1028.6

Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$58,900,000
Sulfuric Acid	\$10,400,000
Caustic	\$43,900,000
Glucose (enzyme production)	\$10,100,000
Hydrogen	\$0
Electricity (import)	\$30,200,000
Other Raw Materials	\$20,000,000
Catalysts	\$800,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$20,900,000
Adipic Acid coproduct (\$0.86/lb)	-\$26,200,000
Fixed Costs	\$22,400,000
Capital Depreciation	\$27,800,000
Average Income Tax	\$8,400,000
Average Return on Investment	\$75,800,000
Total	\$263,100,000

^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)	12.0
Net Electricity Import (kWh/GGE)	17.6
Plant Electricity Use (kWh/GGE)	20.9
Metabolic Yield (g/g substrate)	
Glucose to Butyric	0.465
Glucose to Biomass	0.021
Xylose to Butyric	0.465
Xylose to Biomass	0.021
Arabinos to Butyric	0.140
Arabinos to Biomass	0.021

Appendix B. Life-Cycle Inventory (LCI) for 2019 SOT Benchmark Models

BDO Pathway

	2019 SOT (Burn Lignin)	2019 SOT (Convert Lignin – Base)	2019 SOT (Convert Lignin – High)	
Products				
Production Rate				
Hydrocarbon fuel	9,761	9,778	9,778	kg/hr
	103	104	104	MM kcal/hr (LHV)
Co-products				
Adipic acid (polymer grade)	0	1,736	1,736	kg/hr
Recovered sodium sulfate salt from WWT	9,517	16,175	16,175	kg/hr
Export electricity	-	-	-	kW
Resource Consumption				
Flow Rate (kg/hr)				
Biomass Feedstock (20% moisture)	104,167	104,167	104,167	
Sulfuric acid, 93%	8,753	13,021	13,021	
Caustic (as pure)	6,667	9,922	9,921	
Ammonia	1,305	2,252	2,252	
Glucose	1,589	1,589	1,589	
Corn steep liquor	929	929	929	
Corn oil	9	9	9	
Host nutrients	44	44	44	
Sulfur dioxide	11	11	11	
Diammonium phosphate	100	185	185	
Flocculant	391	391	391	
Toluene solvent makeup	0	0	0	
Hydrogen	789	937	937	
Ethanol	0	13	13	
Boiler chemicals	0	1	1	
FGD lime	111	192	192	
WWT polymer	52	0	0	
Cooling tower chemicals	2	2	2	
Makeup water	145,691	123,275	123,694	
Natural gas for boiler	0	4,700	4,700	
Natural gas for hot oil system	0	0	0	MMBtu/hr
Grid electricity (net import)	19,344	43,228	43,668	kW
Waste Streams				
Flow Rate (kg/hr)				
Disposal of ash	4,293	4,429	4,429	
Air Emissions				
Flow Rate (kg/hr)				
H ₂ O	112,769	101,965	102,031	
N ₂	568,651	437,102	437,068	
CO ₂ (biogenic)	108,732	117,872	117,872	
O ₂	95,553	35,177	35,166	
NO ₂	24	35	35	
SO ₂	7	12	12	
CO	84	60	60	
CH ₄	3	0	0	

Acids Pathway

	2019 SOT (Burn Lignin)	2019 SOT (Convert Lignin – Base)	2019 SOT (Convert Lignin – High)	
Products				
Production Rate				
Hydrocarbon Fuel	9,028	9,028	9,028	kg/hr
	95	95	95	MM kcal/hr (LHV)
Co-products				
Adipic acid (polymer grade)	0	1,760	1,760	kg/hr
Recovered sodium sulfate salt from WWT	9,221	17,049	17,048	kg/hr
Export electricity	-	-	-	kW
Resource Consumption				
Flow Rate (kg/hr)				
Biomass Feedstock (20% moisture)	104,167	104,167	104,167	
Sulfuric acid, 93%	8,753	13,893	13,893	
Caustic (as pure)	6,667	10,586	10,586	
Ammonia	1,310	2,366	2,366	
Glucose	1,589	1,589	1,589	
Corn steep liquor	1,159	1,159	1,159	
Corn oil	9	9	9	
Host nutrients	44	44	44	
Sulfur dioxide	11	11	11	
Diammonium phosphate	150	236	236	
Flocculant	372	372	372	
Toluene solvent makeup	90	90	90	
Hydrogen	0	0	0	
Ethanol	0	13	13	
Boiler chemicals	0	0	0	
FGD lime	113	206	206	
WWT polymer	55	0	0	
Cooling tower chemicals	3	2	2	
Makeup water	340,323	245,405	246,131	
Natural gas for boiler	0	0	0	
Natural gas for hot oil system	38	38	38	MMBtu/hr
Grid electricity (net import)	8,124	55,709	56,146	kW
Waste Streams				
Flow Rate (kg/hr)				
Disposal of Ash	4,296	4,451	4,451	
Air Emissions				
Flow Rate (kg/hr)				
H ₂ O	141,042	99,024	99,091	
N ₂	556,573	637,493	637,518	
CO ₂ (biogenic)	112,415	109,692	109,692	
O ₂	93,834	116,562	116,570	
NO ₂	45	7	7	
SO ₂	8	12	12	
CO	86	34	34	
CH ₄	3	0	0	