

Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2021 State of Technology and Future Research

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National Renewable Energy Laboratory

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List of Acronyms

AD	anaerobic digestion
ANL	Argonne National Laboratory
BCD	base-catalyzed deconstruction (of lignin)
BDO	2,3-butanediol
BETO	Bioenergy Technologies Office
BKA	β-ketoadipate
CEH	continuous enzymatic hydrolysis
ChemCatBio	Chemical Catalysis for Bioenergy Consortium
COD	chemical oxygen demand
CUBI	Catalytic Upgrading of Biochemical Intermediates (under ChemCatBio)
DMR	deacetylation and mechanical refining (pretreatment)
EH	enzymatic hydrolysis
GGE	gallon gasoline equivalent
GHG	greenhouse gas
HDO	hydrodeoxygenation
INL	Idaho National Laboratory
IS	insoluble solids
LCA	life cycle analysis
LHV	lower heating value
LTAD	Low-Temperature Advanced Deconstruction (NREL research project)
MCU	membrane contacting unit
MEK	methyl ethyl ketone
MFSP	minimum fuel selling price
NREL	National Renewable Energy Laboratory
RCD	rotary ceramic disk
ORNL	Oak Ridge National Laboratory
SOT	state of technology
TEA	techno-economic analysis
TS	total solids
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 the National Renewable Energy Laboratory [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 toward out-year goals to ultimately demonstrate cost-competitive cellulosic biofuel technology.

Building upon recent efforts to transition NREL's biochemical platform R&D work toward 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 toward 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 two scenarios for lignin utilization, namely combustion and conversion to value-added coproducts.

A key improvement reflected in the 2021 SOT is centered around making use of the latest lignin conversion data, which over the past year focused primarily on production of β -ketoadipate (BKA) as a more optimal molecule compared to the closely related adipic acid coproduct of prior recent focus, both in terms of superior product properties and biology, as well as reduced processing complexity (reducing two steps for sequential production of muconate followed by hydrogenation to adipic acid down to a single step for direct product output at a nearly fourfold increase in fermentation productivity on lignin monomers relative to prior 2020 SOT benchmarks for muconic/adipic acid production.

Aside from lignin upgrading to coproducts, although further experimental work was performed on other unit operations spanning pretreatment, enzymatic hydrolysis, and sugar fermentation/catalytic upgrading, performance across most of those operations was not observed to surpass levels from the 2020 SOT, and thus 2020 benchmarks were maintained for those operations. For biomass deconstruction to sugars, this included the use of a more optimal twostage deacetylation process preceding mechanical refining, employing sodium carbonate extraction prior to standard sodium hydroxide extraction. This approach was previously shown to enable substantially reduced sodium hydroxide demands, while also translating to very favorable downstream sugar yields from enzymatic hydrolysis at 88% glucan conversion, >93% xylan conversion, and 91% arabinan conversion to monomeric sugars at 10-mg/g enzyme loading. Downstream fermentation metrics were also maintained at 2020 benchmark levels, utilizing over 95% glucose and 89% xylose sugars at fermentation process yields approaching or exceeding future 2030 targets. Catalytic upgrading metrics remained unchanged for the acids pathway, while for the BDO pathway, higher yields and lower costs were demonstrated via improvements in aqueous BDO upgrading space velocity, olefin selectivity, and subsequent olefin oligomerization conversion.

Based on the combination of these process parameter values, the 2021 SOT MFSPs are estimated to be \$6.62/GGE and \$7.07/GGE (\$4.79/GGE and \$5.04/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 42.7 and 38.5 GGE/ton dry biomass for the respective pathways. The 2021 feedstock cost as furnished by Idaho National Laboratory (INL) is \$78.21/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 \$0.18/GGE and \$0.05/GGE in overall MFSPs for the two respective pathways relative to the 2020 SOT.

Alternatively, the SOT scenarios reflecting lignin conversion to coproducts (where the majority of new improvements were focused) indicated MFSP estimates of \$8.65/GGE and \$9.33/GGE for experimental lignin conversion performance on biomass hydrolysate (BDO and acids pathways, respectively). This represents a \$0.69–\$0.82/GGE reduction relative to 2020 SOT benchmarks, attributed to the switch to the more optimal BKA coproduct from bioconversion of lignin monomers in place of muconic/adipic acid, with a sensitivity case indicating that a further \$0.10–\$0.20/GGE reduction would be incurred if BKA could fetch a price premium over adipic acid of 10%–20%, respectively. Still, these results maintain that the lignin-to-coproduct train remains not yet economically profitable relative to burning the lignin, given higher costs for producing the lignin coproduct than the amount of resulting coproduct revenue generated (attributed, in turn, to low—albeit now better—lignin deconstruction/conversion yields and fermentation productivities). This again highlights this process area as a key priority moving forward for future focus in ultimately contributing to MFSP reductions toward 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 2021 SOT Cases Compared to 2017–2020 SOT	а
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	BDO 2017 SOT	Acids 2017 SOT	BDO 2018 SOT	Acids 2018 SOT	BDO 2019 SOT	Acids 2019 SOT	BDO 2020 SOT	Acids 2020 SOT	BDO 2021 SOT	Acids 2021 SOT
	Burn Lignin	Burn Lignin	Burn (Convert)	Burn (Convert)	Burn (Convert)	Burn (Convert)	Burn (Convert)	Burn (Convert)	Burn (Convert)	Burn (Convert)
Minimum fuel selling price (\$/GGE, 2016\$)	\$10.08	\$11.05	\$9.02 (\$12.81)	\$10.40 (\$14.66)	\$7.79 (\$10.80)	\$8.20 (\$11.47)	\$6.80 (\$9.47)	\$7.13 (\$10.02)	\$6.62 (\$8.65)	\$7.07 (\$9.33)
Feedstock contribution (\$/GGE, 2016\$)	\$2.67	\$3.19	\$2.59	\$2.99	\$2.11	\$2.30	\$1.93	\$2.09	\$1.83	\$2.03
Conversion contribution (\$/GGE, 2016\$)	\$7.41	\$7.86	\$6.43 (\$10.22)	\$7.41 (\$11.67)	\$5.67 (\$8.69)	\$5.90 (\$9.17)	\$4.87 (\$7.55)	\$5.04 (\$7.93)	\$4.79 (\$6.82)	\$5.04 (\$7.29)
Hydrocarbon fuel yield (GGE/dry ton)	31.4	26.3	32.3	28	38.5	35.3	41.5	38.5	42.7	38.5

^a 2018–2021 SOT cases: first value in MFSP and "Conversion contribution" lines = burning lignin for heat and power; value in parentheses = converting lignin to coproducts.

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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 is 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 tonnes/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 "nth-plant" production cost for this pre-commercial process.

Recently, the Biochemical Platform Analysis project published the 2018 Biochemical Design Case Update (hereafter referred to as the 2018 design report), which documents 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 considers 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 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 include a deacetylation and mechanical refining (DMR) pretreatment step, followed by wholeslurry batch enzymatic hydrolysis in the diol case or 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 (e.g., adipic acid) 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 2021 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 aforementioned 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 do not yet exist, publicly available information such as that provided in published literature is 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 toward 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 coprocessing 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 are 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 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/blendstocks. 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 and 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):

- DMR step deacetylation/alkaline extraction: While the future target asserts the use of a continuous counter-current alkaline extraction unit as described above and in the design report, experimentally, this step currently maintains standard batch deacetylation as utilized in prior recent SOTs. However, a key update in the present SOT reflects a modification to a *two-step* batch deacetylation approach, adding a sodium carbonate pre-extraction stage prior to the typical sodium hydroxide extraction stage, as a means to reduce sodium hydroxide usage, which has been identified as a key driver in both economic and sustainability metrics.
- 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 maintains standard batch hydrolysis (utilizing the same parameters as in the BDO pathway), followed by the flocculant-assisted vacuum filter press operation to perform in-line solid/liquid separations downstream of batch enzymatic

hydrolysis (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 coproduction 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 and prior SOTs (no hydrogen coproduction).
- 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 vs. acetic acid selectivity in the 2018 SOT to 98% in the 2019–2021 SOTs, 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 prior SOTs, the present analysis again reflects two 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. Additionally, the 2021 SOT update switches to a new, though closely related molecule of interest, now based on β-ketoadipate (BKA) rather than adipic acid as the focus for lignin coproduct valorization. Both fuel pathways consider the following scenarios for lignin utilization:
 - A. Convert lignin under base case conversion parameters observed with actual lignin hydrolysates
 - B. Route all lignin to the boiler to provide more consistent results for comparison with prior SOTs
 - In case #2 (burn lignin), the resulting COD concentration to the wastewater treatment (WWT) system increases as deacetylation black 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 the 2018 design report [2]. Modifications from the 2030 goals as reflected in the current 2021 SOT are denoted in red.

Feedstock

Consistent with prior years, feedstock assumptions for the SOT between 2017 and 2021 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 adjusted 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 2021 SOT, INL achieved a roughly 2% reduction in delivered feedstock cost relative to the 2020 basis, at \$78.21/dry ton inclusive of the above dockage adjustments (personal communication with David Thompson, INL, September 2021).

Table 1. Feedstock Costs Adjusted to 5% Ash for Years 2017–2021 (2016-year dollar	s; courtesy of
David Thompson and Mohammad Roni, INL)	

	2017	2018	2019	2020	2021
Total feedstock cost to biorefinery at 5% ash equivalent (\$/dry ton)	\$83.90	\$83.67	\$81.37	\$80.10	\$78.21
Ash dockage vs. 5% baseline (\$/dry ton) ^a	\$1.26	\$1.24	\$1.58	\$1.39	\$0.38

^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. 2021).

Pretreatment and Enzymatic Hydrolysis

Although new experimental work was conducted over the course of 2021 for biomass deconstruction operations (spanning pretreatment and enzymatic hydrolysis), no new activities were shown to further improve upon the most recent 2020 SOT performance levels. Accordingly, the 2020 benchmarks were maintained in the present update, with key parameters summarized below, followed by a discussion of pertinent experimental activities and findings of note over the past year.

Summary of SOT Input Parameters

Given the recent shift in focus toward 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 fewer 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], batch deacetylation continues to serve as the benchmark operation for SOT purposes 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 batch deacetylation approach as utilized in the prior 2017–2020 SOTs.

However, one key update first incorporated in the 2020 SOT is the addition of a pre-extraction stage prior to the standard sodium hydroxide (NaOH) deacetylation step. This was implemented as an outcome of recent additional focus placed on the substantial usage demands of NaOH and resultant challenges incurred on both economics and more strongly on biorefinery greenhouse gas (GHG) emissions highlighted through life cycle analysis (LCA) modeling. Namely, NaOH usage contributed approximately \$1/GGE to overall MFSP costs in the 2019 SOT ("burn lignin" BDO pathway scenario), roughly \$0.40/GGE of which was subsequently offset by sale of neutralized sodium sulfate salt as a coproduct from wastewater treatment [6]. Likewise, NaOH usage was one of the single largest contributors to overall biorefinery GHG emissions as reflected in Argonne National Laboratory's (ANL's) Supply Chain Sustainability Analysis for the 2019 SOT [7]. Accordingly, in 2020, NREL's Low-Temperature Advanced Deconstruction (LTAD) project focused research efforts on a two-stage deacetylation approach making use of sodium carbonate (Na₂CO₃) as a "sacrificial" alkali material to neutralize acetate and other components of the incoming biomass feedstock, removing the liquor and then subjecting the resultant solids to standard NaOH extraction, followed by mechanical refining and Szego milling ("two-stage DMR").

In the 2020 SOT, the new two-stage DMR approach described above enabled a substantial reduction in NaOH loading relative to prior SOT benchmarks at 80 kg NaOH/dry tonne biomass [8], with an optimal case identified at a Na₂CO₃ and NaOH loading of 80 and 24 kg/dry tonne biomass, respectively, with each step performed sequentially at 90°C and 2-hour batch time. This translated to 88% and 93% conversions of glucan to glucose and xylan to xylose, respectively, demonstrated using a favorable enzyme loading of 10 mg/g cellulose (8 mg cellulase and 2 mg hemicellulase enzymes) at 20% total solids loading. The two-stage deacetylation operation produced a black liquor product containing roughly 13% of the original biomass xylan, 3% of the glucan, 48% of the arabinan, 11% of the ash, and 100% of the acetates, along with solubilizing 20% of the biomass lignin. In the "convert lignin" scenarios for adipic acid coproduction, 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 [2, 9]. The power for the subsequent mechanical refining step was set at 200 kWh/dry ton biomass, consistent with vendor inputs provided previously [10].

Discussion of Latest R&D Activities and Future Plans

In 2021, research under the LTAD project focused on reducing mechanical refining energy through optimization of the refining conditions. In DMR pretreatment, mechanical refining is used to delaminate and defibrillate lignocellulosic biomass to facilitate enzyme access without introducing inhibitors for downstream processes. While multiple stage refining may be employed

using different machines, disc refining is the principal and crucial step that overcomes the biomass recalcitrance mainly by three biomass structural disruption mechanisms: external fibrillation, internal delamination, and fiber cutting. Disc refining has demonstrated its capability in increasing surface area accessible to enzymes and improving carbohydrate conversion through the disruption of biomass structure, including size reduction and fibrillation. However, disc refining is an effective but energy-intensive technology, with about 20%–30% of the total energy used in the DMR pretreatment. The energy consumption-related GHG emissions are critical for the success of a DMR process-based cellulosic biofuel economy, considering GHG emissions caused by the mechanical refining energy usage. By using a 12" disk refiner at NREL, promising energy reduction was achieved by optimizing refining conditions and improving plate designs of refining disks without sacrificing sugar yields. One plate showed similar glucose yield (79.5%) compared to another plate (84.3%) with 43% energy reduction. Although more research is needed to improve xylose yield at lower refining energy, this research will eventually lead to better refining plate designs and optimization for larger-scale refiners to reduce refining energy-related GHG emissions.

Further optimization on two-stage deacetylation conditions is also ongoing under the LTAD project. A central composite design of experiment has been carried out to improve sugar yields and reduce the pretreatment chemical-related GHG emissions by screening for optimal loadings of sodium carbonate and sodium hydroxide. An optimization model has been developed, predicting that 90% glucose yield and 90% xylose yield could occur at higher sodium carbonate and lower sodium hydroxide loadings than evaluated in the prior SOT.

The Continuous Enzymatic Hydrolysis Development project continues to focus on reducing GHG emissions by increasing processing efficiency, improving the economics, and reducing scale-up risks of biorefinery sugar-lignin production through development of a deployable CEH process. Cost advantages of continuous biochemical deconstruction implemented via a combined DMR + CEH pretreatment + enzymatic hydrolysis approach include: enabling a continuous biomass sugars-lignin manufacturing platform; reducing sugar product feedback inhibition on the EH reaction to achieve higher sugar conversion and recovery yields and potentially also higher productivity; facilitating downstream upgrading strategies that require clarified sugar streams (such as for aqueous inorganic catalysis and certain bio-upgrading strategies such as extractive fermentation), as well as lignin streams unadulterated by polyelectrolyte flocculants; and consolidation of unit operations required to produce a concentrated clarified sugars stream. TEA of an envisioned multistage CEH process shows that economics are a strong function of CEH membrane performance and membrane circulation loop energy requirements (i.e., energy for pumping biomass enzymatic hydrolysis slurries). The end-of-project target is to demonstrate a 20% improvement in projected CEH cost relative to conventional batch EH followed by solidliquid separation. These more favorable economics are expected to able to be achieved through optimization of multistage CEH processing by using an optimal number of CEH stages (reactormembrane units) and potentially by excluding ex situ solid-liquid separation in one or more stages. Alternative membrane materials and lower-cost membranes, as well as refined CEH configurations, also offer opportunities to improve CEH process costs.

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 BDO fermentation data were maintained reflecting 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 finer 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/m²-h, 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 [11]. 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

Similar to the pretreatment/hydrolysis steps, while further experimental work was conducted over the course of 2021 for the fermentation and catalytic upgrading operations under both fuel pathways, the majority of these activities did not ultimately lead to quantifiable improvements as modeled in the SOT relative to prior benchmarks, with the exception of catalytic upgrading for the BDO pathway. However, important learnings were still made regarding implications for process integration and scale-up. Key details for these steps are summarized below, along with a brief discussion of the activities performed and insights gained in the relevant tasks.

Summary of SOT Input Parameters

In the acids pathway, the clarified hydrolysate is routed to sugar concentration, 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 coproduced at a roughly 50:1 mass ratio (less than 2 wt % acetic acid) using Clostridium tyrobutyricum. This was coupled with pertractive recovery of the acids as a key approach to maintaining economic viability compared to pH-controlled fermentation with significant amounts of added caustic and subsequent salt disposal costs. In contrast to earlier SOT experimental efforts, which generally performed acid fermentation in batch mode with separate operations to demonstrate fermentation and pertractive acid recovery in isolation, the 2019–2021 SOT efforts were done in a physically integrated system, with fermentation operated in fed-batch mode, coupled with continuous recovery of acids across a pertraction membrane. The conversion of sugars to products was maintained consistent with the 2020 SOT at 95% glucose (demonstrated) and 95% xylose (not fully demonstrated given logistical decisions for how the fed-batch system was operated with in situ acid removal, but expected to be realistic), with an additional 2.5% conversion to cell biomass for glucose/xylose and 9% for arabinose. Additionally, arabinose conversion to product was maintained at 20%, although a caveat is added here that while arabinose consumption has

been observed, more recent experimental work suggests the organism may not actually be converting it to butyric acid (further work is planned to investigate this, but MFSP impacts are minimal at 20% conversion for this minor sugar). Fermentation productivity was also maintained at 0.62 g/L-h.

Recovery of acids was also set consistent with prior recent SOTs at 98.4% and 76.4% for butyric and acetic acids, respectively, based on a solvent system composed of 20% tri-octyl-phospheneoxide (TOPO) plus 40% undecanone in mineral oil. In the 2019–2021 SOT models, distillation is employed to boil the acids off from the heavier-boiling solvents as the commercially practical approach relative to use of NaOH back-extraction (given known significant penalties incurred with the required levels of NaOH to perform this operation). The recovered acids are next subjected to catalytic upgrading, based on prior SOT data furnished by NREL researchers under the Chemical Catalysis for Bioenergy Consortium (ChemCatBio) Catalytic Upgrading of Biochemical Intermediates (CUBI) efforts. In brief, acid substrate first undergoes ketonization over a ZrO₂ catalyst at 4 h^{-1} weight hourly space velocity (WHSV) and 435°C, achieving 100% acid conversion with 93% selectivity to 4-heptanone (adjusted in the model to complete conversion to 4-heptanone given indications that the remainder follows a similar fate as 4heptanone in downstream steps). 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 similar to prior years, including use of a slurry reactor utilizing a Nb₂O₅ catalyst at a ratio of 1:4 wt catalyst:ketone, 10-hour residence time, and toluene solvent at a loading of 4:1 wt toluene:ketone, resulting in an overall process yield of 92 wt % to enone products from feed ketones (after recycling unconverted ketones). Finally, the enone intermediates are upgraded to hydrocarbons via hydrodeoxygenation (HDO), again largely maintaining consistent details as prior SOTs including use of a 3% Pt/Al₂O₃ catalyst at a WHSV of 4.7 h⁻¹ and temperature of 334°C, achieving 100% conversion to products (primarily C14 branched hydrocarbon from the C14 enone).

For the BDO pathway, additional fermentation runs were conducted in 2021, primarily investigating possibilities for achieving higher BDO titers beyond the prior SOT benchmark of 70 g/L. As that prior benchmark reflected already very high sugar conversions to BDO based on batch fermentation, the ability to push BDO titers higher would require either (1) starting with more concentrated sugars in whole-slurry hydrolysate (in turn implying higher solids loadings through upstream enzymatic hydrolysis); (2) moving to fed-batch fermentation feeding clarified, concentrated sugars; or (3) an alternate fermentation configuration. To date, option (1) has proven challenging as initiating batch fermentation with high sugar concentrations over approximately 150 g/L leads to osmotic shock for the cells, while option (2) would add substantial cost and energy penalties for a concentration step not otherwise utilized in the BDO pathway schematic. Accordingly, the final option was considered as a primary focus area during 2021, namely evaluation of an alternative configuration based more on a simultaneous saccharification and fermentation (SSF) mode of operation, whereby enzymatic hydrolysis is initiated and fermentation commences as sugar concentration builds, after which point more solids with additional enzyme are added in a fed-batch mode, providing additional sugars that are consumed through fermentation as they are produced from enzymatic hydrolysis. While this approach was able to achieve a titer over 100 g/L of combined BDO and acetoin, it did so at the expense of low overall yields (roughly 54% overall conversion of carbohydrates to BDO) and high enzyme loading (approximately 25 mg/g cellulose) given suboptimal temperature and pH

conditions for achieving good enzymatic hydrolysis. Thus, the SOT model maintained the use of prior benchmarks with batch fermentation, reflecting nearly 100% overall glucose utilization and 92% xylose utilization at 97% metabolic yield to BDO within 48 hours (roughly 1.4 g/L-h productivity). 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.

Following BDO fermentation, the fermenter broth is first clarified in a lignin press (consistent with that used in prior ethanol work) and then sent to polishing filtration, assumed to be two parallel skid units made up of microfiltration, nanofiltration, and ion exchange, including cleanin-place systems and backwash, before being routed to catalysis steps. For BDO catalytic upgrading, new experimental data furnished by Oak Ridge National Laboratory (ONRL) collaborators under support of the CUBI consortium were incorporated. Three data sets were provided representing high/low, medium/medium, and low/high selectivities for aqueous BDO conversion to C3+ olefins versus methyl ethyl ketone (MEK). Although MEK could be isolated and sold as an additional coproduct, this SOT maintains a focus on maximizing fuel yield from the carbohydrate fraction. Thus, the high olefin case was selected, achieving 100% BDO conversion with 69% yield to olefins and 30% to MEK; this was comparable to prior SOT benchmarks with 68% yield to olefins and 28% to MEK, but also now achieving a doubling in WHSV at 2.0 h⁻¹ versus 1.0 h⁻¹ previously, based on a copper-based zeolite catalyst (Cu/PMFI) at 250°C. Additionally, after purifying the resultant olefin products by distillation, subsequent oligomerization conversions were also adjusted from 95% C3/C4 and 100% C5/C6 olefin conversion to 100% and 95%, respectively, based on the latest ORNL data which indicates complete conversion of propene and butenes (the majority olefin components from the BDO conversion step). The resultant oligomers (generally C4–C20 olefins) are then hydrotreated to hydrocarbon fuels.

Discussion of Latest R&D Activities and Future Plans

Under the Biological Upgrading of Sugars project, research has focused on three major topics for carboxylic acid fermentation: (1) acquiring the components of the pilot-scale reactor and undertaking process hazard assessment, (2) further optimizing bench-scale fermentations, and (3) generating molecular genetic tools and developing superior strains for fermentation. We have now acquired all major components of the pilot reactor including rotary ceramic disk filtration unit, progressing cavity pumps, membrane contactors, and a flash distillation unit. Furthermore, we anticipate finalizing the process hazard assessments of every system in the near future. This will enable us to finalize design and construction of the reactor in 2022. Related to fermentation optimization, we have negotiated and acquired a suite of novel organic extractants for the in situ product recovery system, which we hypothesize will have equivalent extraction abilities with a reduced biological toxicity. Such an extractant will improve our overall process metrics, and we will be evaluating these in early 2022. Related to strain improvement activities, we have generated a series of strains through both rational engineering and mutagenic approaches. Areas that we have focused on include improved tolerance to low pH, which will enhance acid pertraction; increased ability to utilize xylose; increased tolerance to butyrate; and increased tolerance to organic extractants. We have several lineages of promising strains that are currently being evaluated. Two lineages that are particularly promising are a collection of mutants capable of growth at pH 4.5 and a collection of mutants with greatly improved xylose utilization. We are currently evaluating these strains to assess their capabilities in bioreactors. Additional

collaborations with the Agile BioFoundry are rapidly improving our ability to generate improved strains in a shorter period of time, and we anticipate this collaboration will expand in 2022.

In 2021, the separations group conducted research to address the most capital cost-intensive equipment associated with the *in situ* product recovery system as a means to lower the cost of the butyric-acid-to-fuel pathway. In this system, sterile filtered permeate from a rotary ceramic disk (RCD) laden with butyric acid is passed through a membrane contacting unit (MCU). The MCU is a commercially available unit consisting of polypropylene hollow fibers. The MCU is used to increase surface area contact between the organic extractant (Cyanex 923) and aqueous phase, increasing the rate of extraction approximately one thousandfold over a simple organic overlayer setup. Cyanex is recirculated through the tube side of the MCU counter current to the aqueous phase on the shell side, selectively extracting the acids through hydrogen bonding. After extraction, the more volatile acids and a small amount of co-extracted water (~5–10 wt %) are stripped from the high-boiling Cyanex by flash distillation, with the recovered Cyanex recycled back to the MCU. Water and acids are then separated in a four-stage polishing column. Overall, this system allows continuous extraction of butyric acid from a bioreactor under favorable energy demands, but is capital-intensive, primarily for the RCD and MCU operations. To lower these large capital expenses, a new process approach is being considered to replace the RCD with a different dynamic vibrating membrane filter referred as the VSEP unit. The VSEP unit is available commercially at industrial scale, at roughly one-fourth the cost of the RCD. To lower the cost of the MCU, a membrane-based emulsion separator is proposed. Here, permeate from the VSEP that is laden with butyric acid is mixed in line with the Cyanex extractant that selectively extracts the acids. The emulsion is rapidly separated with a membrane separator, which exploits the interfacial tension between the two phases to break the emulsion, requiring less than 10 times the area of the MCU to achieve the required separation. Initial TEA work done under the Separations Consortium has found this alternative processing approach to enable a roughly 60% reduction in capital cost and 25% reduction in operating cost per ton of butyric acid produced, which may be leveraged in future SOTs to further reduce the MFSP relative to current benchmarks.

Under CUBI efforts for carboxylic acid upgrading, research activities focused on evaluating the rate law for short-chain acid ketonization using a downselected commercial ZrO₂ catalyst provided by Johnson Matthey. At high acid partial pressures, the ketonization rate was determined to be zero-order in acid concentration, with no rate inhibition observed with the product ketone or CO₂. Water partial pressure was shown to inhibit the ketonization rate, with work next year planned to evaluate reactor configurations to knock out water and minimize rate inhibition. The heat of reaction was determined to be mildly endothermic, with modeling calculations suggesting limited heat- and mass-transfer impacts when transitioning to pelletized catalyst materials. To reduce the cost of hydrodeoxygenation, catalytic tests were also performed with commercial NiMo/Al₂O₃ pellets that would be 1/20 the price of the baseline Pt/Al₂O₃ catalyst. Complete deoxygenation of the model ketone, 6-undecanone, was observed with crushed NiMo/Al₂O₃ pellets under relatively mild conditions (350°C, 1,000-psig H₂), and little to no cracking or isomerization products were observed. Work next year will evaluate the rate and stability of NiMo/Al₂O₃ for ketone hydrodeoxygenation during continuous operation for at least 24 hours of time on stream. Lastly, jet fuel property testing was performed under the Opportunities in Biojet program. Results confirmed that sustainable aviation fuel produced from

short-chain acids can meet ASTM fuel property requirements, with final jet fuel blend properties highly dependent on the short-chain acid carbon number distribution [12].

Finally, in the bench-scale R&D project, a research focus is to produce high titers of BDO from fermentation to reduce the amount of water processed in downstream separations and upgrading. In 2020, we were successful in hitting a 125-g/L BDO titer goal using concentrated biomass liquor that does not contain solids. In 2021, we worked on a whole-slurry fermentation that pushed the concentration of whole-slurry solids to above 25% w/w solids, with the goal of 100g/L BDO titer using our 500-mL benchtop bioreactors. We were met with numerous challenges as we increased solids: needing to feed solids in a fed-batch configuration to avoid an initial sugar concentration above 150 g/L, which inhibits the biocatalyst; mixing challenges due to high solids, which alter the oxygen mass-transfer rate and affect the products produced; and enzymatic hydrolysis at fermentation conditions not optimal for the enzyme. Despite these challenges, our current results yielded 100 g/L of upgradeable products (70-g/L BDO and 30-g/L acetoin) and 83% fermentation process yield. While we could show 100-g/L upgradeable products from whole-slurry DMR, the poor enzymatic hydrolysis yields, unconverted xylose, and high acetoin levels warrant more work on optimizing the fermentation conditions for the higher solids needed to achieve the higher BDO titer. Moving forward, we plan to explore using sorbitol for higher-sugar batch fermentations to avoid feeding solids. We plan to reoptimize the aeration levels for DMR solids to reduce the acetoin levels, keep glycerol low, and increase BDO. We are also looking at increasing enzyme loading for the purpose of demonstrating the whole-slurry fermentation process. A higher enzyme loading would increase sugar concentrations at lower solids, which would improve the bench-scale fermentor operations, though this would have to be weighed against the economics to optimize overall enzyme levels and associated yields.

Lignin Utilization

Relative to prior SOT benchmarks, the 2021 SOT incorporates new data for a modified lignin utilization approach reflecting the latest focus of experimental efforts, namely shifting from two-stage bioproduction of muconic acid and subsequent upgrading to adipic acid to single-stage bioproduction of BKA. Again, key SOT input parameters as utilized for the present SOT are briefly summarized below, followed by a discussion on other recent lignin upgrading activities and accomplishments.

Summary of SOT Input Parameters

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. 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, maintaining all parameters for BCD consistent with prior SOTs. Bench-scale results have indicated 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).

Experimental work in 2021 focused primarily on bioconversion of lignin monomers to BKA, building on prior recent experimental and TEA modeling work demonstrating superior

fermentation performance and economics for BKA production from *Pseudomonas putida* than adipic acid, with concomitantly superior properties as a performance-advantaged bioproduct [13, 14]. On the latter point, the addition of the β -ketone into the adipic acid molecule structure was found to enable superior thermal properties for nylon-6,6, a key derivative product, when synthesized from BKA in place of adipic acid, while enabling favorable carbon intensity compared to traditional adipic acid production [13, 14]. The BKA fermentation step itself was maintained identical to prior TEA modeling details described for muconic acid fermentation, based on fed-batch fermentation of aromatic lignin monomers available in the hydrolysate substrate [2].

The experimental campaign achieved a BKA yield of 1.13 mol BKA/mol lignin aromatics in DMR black liquor with >100% yield, indicating conversion of higher-molecular-weight lignin or other uncharacterized compounds, thus essentially improving molar yield to the fermentation product by 13% relative to prior SOT benchmarks at 100% conversion of lignin monomers to muconic acid. Additionally, fermentation productivity (known to be a crucial driver on overall economics at the low historical SOT values below roughly 0.3 g/L-h [15]) was shown to increase fourfold, from 0.06 g/L-h in previous SOTs with muconic acid to 0.23 g/L-h with BKA. Given limited resources, these performance data for BKA production were based only on conversion of the DMR black liquor material, but with prior work consistently demonstrating similar performance for BCD liquor as DMR liquor, the same performance parameters were assumed here for the additional liquor stream produced following residual solids BCD. Downstream of fermentation, the BKA process differs from the prior muconic/adipic acid schematic, which underwent acidification, low-pH crystallization of muconic acid, hydrogenation to adipic acid, and further crystallization of the final adipic acid product [2]; rather, in this case, the BKA product is purified using similar equipment as that described in prior NREL TEA work for succinic acid production [16], namely acidification and simulated moving bed ion exchange. For this assessment, the BKA coproduct value was assumed to be the same as that of adipic acid, set at \$0.86/lb based on prior TEA models representing a multiyear average market price. If anything, this likely errs on the conservative side given the superior properties for downstream product synthesis imparted by BKA versus adipic acid; thus, higher potential values are also considered as a sensitivity case.

Discussion of Latest R&D Activities and Future Plans

In 2021, the Lignin Utilization project developed a chemo-catalytic method to oxidatively cleave C–C bonds to produce higher yields of bioavailable monomers than are present in the streams where C–O bond cleavage alone has been achieved. This work will enable a higher theoretical yield of muconic acid and β –ketoadipic acid from oligomeric lignin beyond 2021. This work will be reported in early 2022.

Additionally, work in the Separations Consortium has resulted in the ability to conduct molecular weight fractionation of lignin streams, including alkaline pretreated liquor, with low energy input and costs that are feasible for downstream bioconversion into the same products. This work has been reported in previous milestones and is the subject of a peer-reviewed manuscript under preparation.

Additionally, the Lignin-First project has made major strides in TEA and LCA of an alternative reductive catalytic fractionation (RCF) process, which holds promise to enable woody feedstocks

in biochemical conversion processes that the DMR-EH process cannot currently handle. We reported a comprehensive TEA and LCA that highlights solvent recovery, reactor pressure, and residence time as major cost, energy, and GHG drivers [17]. The Lignin-First Biorefinery Development Project is now working with two industrial partners and closely with the Separations Consortium team with a focus on developing robust bench-scale technology and to scale up the RCF process as a promising alternative to standard thermochemical pretreatment technologies that places lignin on an equal footing to carbohydrates from a valorization perspective. We have achieved solvent loadings of 3 L solvent/kg biomass in a specialized reactor setup, which is substantially lower than has been achieved in batch reactors previously.

In parallel to these efforts, the Biological Lignin Valorization project has initiated the evaluation of the performance of Pseudomonas putida in depolymerized lignin streams generated in the Lignin Utilization project and streams generated from fractionation processes in the Separations Consortium. These initial campaigns are critical to identify potential bottlenecks that need to be overcome to improve the biocatalyst performance. The Biological Lignin Valorization project has also continued developing bioprocesses to increase muconate and ß-ketoadipate titers, yields, and productivity from lignin-derived monomeric aromatic compounds and lignin streams from the DMR process. An exemplary data set from aromatic compounds in 2021 was related to the significantly increased productivity of B-ketoadipate from p-coumarate by engineered P. putida (up to 1.1 g/L/h) while achieving titers of 44 g/L at a yield of 0.93 mol/mol. Regarding the lignin, the effect of feeding solids (dried DMR black liquor) in fed-batch mode and as the sole carbon source was also tested. The purpose of these experiments was to achieve higher concentrations of aromatic compounds in the feeding to increase product titers and productivity and, consequently, to improve the SOT benchmark. As hypothesized, the baseline ß-ketoadipate titers were increased up to 5 g/L, and most importantly, the productivity was enhanced fourfold, up to 0.23 g/L/h. Because these lignin streams contain high salt concentrations, strain development will also focus on improving the responses to osmotic stress.

Results

TEA Results

Based on the details summarized above for experimental performance across the integrated processes, the 2021 SOT benchmark for the **BDO pathway ("burn lignin" scenario)** is estimated at an overall MFSP of **\$6.62/GGE total or \$4.79/GGE for conversion-related costs (2016 dollars)** excluding feedstock allocations, with feedstock cost set at \$78.21/dry ton, associated with a 5% ash-equivalent biomass composition as described previously. This corresponds to an overall fuel yield of 42.7 GGE/ton biomass (24.5% 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 \$0.18/GGE (3%) lower MFSP relative to last year's 2020 SOT case for the BDO pathway (\$6.80/GGE in 2016 dollars) when viewed on comparable footing (i.e., based also on burning lignin in the 2020 case), enabled by improvements in the BDO upgrading catalyst details as well as marginal feedstock cost improvements discussed above.

Similar to the findings in last year's 2020 SOT, the 2021 SOT yield and MFSP results remain 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 deacetylation and dilute acid 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 toward 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 \$8.65/GGE for BKA fermentation performance on hydrolysate. These results are associated with roughly 85% solubilization of residual solid lignin recovered from downstream processing, 18% of which is convertible across lignin fermentation at a BKA process yield of 0.19 g/g total soluble lignin. Given the low fraction of convertible species in the solubilized lignin material, the overall lignin coproduct yields are roughly 18% of their final 2030 targets (on a mass basis), which combined with 77% lower fermentation productivities (and accordingly higher fermentation/processing costs) continues to translate to a *net cost penalty* when lignin coproducts are included, reflecting higher costs to produce the coproduct than the revenue it generates. However, although lignin upgrading has still not yet reached an economic breakeven point with combustion, the switch to BKA production enabled a net MFSP reduction of \$0.82/GGE (9%) for the 2021 SOT BDO pathway relative to prior 2020 SOT values for the lignin conversion scenario.

Utilizing the inputs from experimental work for the **carboxylic acids pathway ("burn lignin" scenario**), an overall MFSP of **\$7.07/GGE total or \$5.04/GGE for conversion-related costs (2016 dollars)** excluding feedstock allocations is estimated for the 2021 SOT. This corresponds to an overall fuel yield of 38.5 GGE/ton biomass (22.5% 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. This result is slightly lower than the 2020 SOT baseline at \$7.12/GGE, strictly as a function of lower feedstock cost (as discussed above, no further improvements were made to the fuel-relevant operations in the acids pathway outside of lignin coproduct upgrading). For the alternative acids pathway SOT scenarios reflecting **lignin utilization**, the **MFSP is estimated at**

\$9.33/GGE for BKA fermentation performance, based on maintaining the same lignin deconstruction and conversion parameters as noted above for the BDO case. Compared with the 2020 SOT results for the "base case" lignin coproduct scenario producing adipic acid, this leads **to reductions of \$0.69/GGE (7%)**, again enabled by the switch to the higher-yield, higher-productivity, lower-complexity BKA coproduct in place of two-stage muconic/adipic acid production.

As noted above, the BKA coproduct was conservatively assumed to reflect a market value consistent with that used in historical TEA models for adipic acid (\$0.86/lb) given the similarities and common primary end use (nylon) for either product. However, as BKA ultimately is viewed as a superior molecule with the ability to impart better properties in the resultant end product described previously, a sensitivity case was evaluated at higher market values relative to the adipic acid baseline. At a **10% price premium for BKA** (\$0.94/lb), the resultant **lignin utilization MFSPs would reduce to \$8.55/GGE for the BDO pathway or \$9.23/GGE for the acids pathway**, while at a **20% premium** (\$1.03/lb), the **MFSP would reduce further to \$8.46/GGE or \$9.12/GGE, respectively**. Although these impacts to MFSP are somewhat modest at current SOT yield levels for the BKA coproduct, the impact would become substantially more pronounced with more dramatic MFSP savings in a future case—i.e., given 2030 target lignin coproduct yields over fivefold higher than current SOT benchmarks.

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2030 Proiection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: BKA ª	Convert Lignin
Projected minimum fuel selling price	\$/GGE	\$10.08	\$9.02	\$12.81 (\$11.54)	\$7.79	\$10.80 (\$9.72)	\$6.80	\$9.47 (\$8.62)	\$6.62	\$8.65	\$2.47
Feedstock contribution	\$/GGE	\$2.67	\$2.59	\$2.59	\$2.11	\$2.11	\$1.93	\$1.93	\$1.83	\$1.83	\$1.65
Conversion contribution	\$/GGE	\$7.41	\$6.43	\$10.22 (\$8.95)	\$5.67	\$8.69 (\$7.61)	\$4.87	\$7.55 (\$6.70)	\$4.79	\$6.82	\$0.82
Total gasoline equivalent yield	GGE/dry U.S. ton	31.4	32.3	32.3	38.5	38.5	41.5	41.6	42.7	42.9	43.2
Adipic acid [BKA] coproduct yield	lb/dry ton biomass	0	0	40	0	42	0	39	0	[47]	266
Feedstock	,										
Feedstock cost ^b	\$/dry U.S. ton	\$83.90	\$83.67	\$83.67	\$81.37	\$81.37	\$80.10	\$80.10	\$78.21	\$78.21	\$71.26
Pretreatment					-						
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids loading	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	90	90	90	90	90	90	92
Reactor mode	Batch vs. counter- current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter- current
Total loading: NaOH [Na ₂ CO ₃]	mg/g dry biomass	70	70	70	80	80	24 [80]	24 [80]	24 [80]	24 [80]	70
Net solubilized lignin to liquor	%	47%	47%	47%	50%	50%	20%	20%	20%	20%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	3%	3%	3%	3%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	16%	16%	12%	12%	12%	12%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	48%	48%	48%	48%	30%
Enzymatic Hydrolysis											
Hydrolysis configuration	Batch vs. CEH	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch
Total solids loading to hydrolysis	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	25%
Enzymatic hydrolysis batch time	days	5	5	5	5	5	7	7	7	7	5
Hydrolysis glucan to glucose	%	78%	78%	78%	84%	84%	88%	88%	88%	88%	90%
Hydrolysis xylan to xylose	%	85%	85%	85%	82%	82%	93%	93%	93%	93%	90%
Sugar loss (into solid stream after EH separation)	%	5%	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)	N/A (whole slurry)
Cellulase Enzyme Production											
Enzyme loading	mg/g cellulose	12	12	12	12	12	10	10	10	10	10
Fermentation, Catalytic Conversion, and	Upgrading to Fuels										
Bioconversion volumetric productivity	g/L/hour	1.7	1.1	1.1	1.43	1.43	1.43	1.43	1.43	1.43	2.6
Glucose to product [total glucose utilization] °	%	86% [100%]	95% [100%]	95% [100%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	95% [98%]
Xylose to product [total xylose utilization] $^{\circ}$	%	89% [97%]	90% [92%]	90% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	90% [92%]

Table 2(a). BDO Pathway: Technical Summary Table for 2021 SOT Benchmark, 2017–2020 Back-Cast SOT, and Future 2030 Targets [2]

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin: Base (High) ^a	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: BKA ª	Convert Lignin
Arabinose to product [total arabinose utilization] °	%	0% [0%]	0% [0%]	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]	0.47 [0.44]	0.47 [0.44]	0.47 [0.45]	0.47 [0.45]	0.47 [0.45]	0.47 [0.45]	0.47 [0.45]	0.47 [0.45]	0.47 [0.45]
Fermentation intermediate product recovery	wt %	99.7%	96.8%	96.8%	97.7%	97.7%	97.7%	97.7%	97.7%	97.7%	96.4%
Aqueous BDO upgrading: WHSV	h ⁻¹	1	1	1	1	1	1	1	2	2	2
Aqueous BDO upgrading: per-pass conversion	wt % to desired products	89%	90%	90%	100%	100%	100%	100%	100%	100%	100%
Oligomerization: WHSV	h ⁻¹	1	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%	100%	100%
Hydrotreating: WHSV	h⁻¹	5	5	5	5	5	5	5	5	5	5
Hydrotreating: per-pass conversion	wt % to desired products	100%	100%	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%	-	18%	98%
Fermentation process yield from lignin	g/g soluble lignin	-	-	0.15	-	0.16	-	0.16	-	0.19	1.59
Fermentation metabolic yield from lignin	g/g lignin consumed	-	-	0.93	-	0.93	-	0.93	-	1.19	0.93
Overall carbon upgrading efficiency to coproduct ^d	mol %	-	-	3.8%	-	3.8%	-	4.0%	-	5.4%	27.8%
Fermentation productivity	g/L/h	-	-	0.06 (0.53)	-	0.06 (0.53)	-	0.06 (0.53)	-	0.23	1
Coproduct production	MMlb/yr	-	-	29	-	30	-	29	-	34	193

^a 2018–2020 lignin conversion "base" case from actual black liquor/BCD hydrolysate; "high" case (in parentheses) = highest productivity observed to date based on model lignin monomers. 2021 lignin conversion to BKA only reflected actual hydrolysate (akin to "base" case previously).

^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 brackets indicate total sugar utilization (including biomass organism propagation).

^d Includes fermentation of all convertible components, plus product recovery and subsequent upgrading (adipic acid cases)

^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 lignin coproduct.

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: BKA ^a	Convert Lignin
Projected minimum fuel selling price	\$/GGE	\$11.05	\$10.40	\$14.66 (\$13.16)	\$8.20	\$11.47 (\$10.29)	\$7.13	\$10.02 (\$9.04)	\$7.07	\$9.33	\$2.49
Feedstock contribution	\$/GGE	\$3.19	\$2.99	\$2.99	\$2.30	\$2.30	\$2.08	\$2.09	\$2.03	\$2.04	\$1.59
Conversion contribution	\$/GGE	\$7.86	\$7.41	\$11.67	\$5.90	\$9.17	\$5.04	\$7.93	\$5.04	\$7.29	\$0.90
Total gasoline equivalent yield	GGE/dry U.S. ton	26.3	28	(\$10.17) 28	35.3	(\$7.98) 35.3	38.5	(\$6.96)	38.5	38.4	44.8
Adipic acid [BKA] coproduct vield	lb/dry ton biomass	0	0	41	0	42	0	40	0	[48]	259
Feedstock	is ally ton signate	0	0		0	12	Ū	10	0	[10]	200
Feedstock cost ^b	\$/dry U.S. ton	\$83.90	\$83.67	\$83.67	\$81.37	\$81.37	\$80.10	\$80.10	\$78.21	\$78.21	\$71.26
Pretreatment	·										
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids loading	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	90	90	90	90	90	90	92
Reactor mode	Batch vs. counter- current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter- current
Total loading: NaOH [Na ₂ CO ₃]	mg/g dry biomass	70	70	70	80	80	24 [80]	24 [80]	24 [80]	24 [80]	70
Net solubilized lignin to liquor	%	47%	47%	47%	50%	50%	20%	20%	20%	20%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	3%	3%	3%	3%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	16%	16%	12%	12%	12%	12%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	48%	48%	48%	48%	30%
Enzymatic Hydrolysis											
Hydrolysis configuration	Batch vs. CEH	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	CEH
Total solids loading to hydrolysis	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	7.60%
Enzymatic hydrolysis batch time	days	5	5	5	5	5	7	7	7	7	Continuous
Hydrolysis glucan to glucose	%	78%	78%	78%	84%	84%	88%	88%	88%	88%	96%
Hydrolysis xylan to xylose	%	85%	85%	85%	82%	82%	93%	93%	93%	93%	99%
Sugar loss (into solid stream after EH separation)	%	5%	5%	5%	5%	5%	5%	5%	5%	5%	1%
Cellulase Enzyme Production											
Enzyme loading	mg/g cellulose	12	12	12	12	12	10	10	10	10	10
Fermentation, Catalytic Conversion, and	Upgrading to Fuels										
Bioconversion volumetric productivity	g/L/hour	1.1	0.3	0.3	0.62	0.62	0.62	0.62	0.62	0.62	2
Glucose to product [total glucose utilization] $^{\circ}$	%	86% [100%]	90% [95%]	90% [95%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [100%]
Xylose to product [total xylose utilization] °	%	82% [100%]	77% [90%]	77% [90%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	85% [100%]

Table 2(b). Acids Pathway: Technical Summary Table for 2021 SOT Benchmark, 2017–2020 Back-Cast SOT, and Future 2030 Targets [2]

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2030 Projection
Lignin Handling	-	Burn Lignin	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: Base (High) ª	Burn Lignin	Convert Lignin: BKA ^a	Convert Lignin
Arabinose to product [total arabinose utilization] $^{\circ}$	%	82% [100%]	32% [38%]	32% [38%]	20% [29.0%]	20% [29.0%]	20% [29.0%]	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 [0.44]	0.45 [0.44]	0.45 [0.44]	0.45 [0.44]	0.45 [0.44]	0.45 [0.44]	0.45 [0.43]
Fermentation intermediate product recovery	wt %	60% (C2), 95% (C4)	60% (C2), 95% (C4)	60% (C2), 95% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	76% (C2), 98% (C4)	100% (C4)
Ketonization: WHSV	h⁻¹	6	4	4	4	4	4	4	4	4	6
Ketonization: per-pass conversion	wt % to desired products	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Condensation: WHSV	h ⁻¹	0.5	10-h residence time	10-h residence time	10-h residence time	10-h residence time	10-h residence time	10-h residence time	10-h residence time	10-h residence time	15-h batch
Condensation: overall conversion	wt % to desired products	81%	92%	92%	92%	92%	92%	92%	92%	92%	60% pp
Hydrotreating: WHSV	h⁻¹	3	4.7	4.7	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%	100%	100%
Lignin Processing to Coproduct											
Solid deconstruction to soluble lignin	wt % BCD lignin feed	-	-	85% ^e	53%						
Convertible components in soluble lignin	wt % of total soluble lignin (APL + BCD)	-	-	16%	-	16%	-	16%	-	18%	98%
Fermentation process yield from lignin	g/g soluble lignin	-	-	0.15	-	0.16	-	0.16	-	0.19	1.59
Fermentation metabolic yield from lignin	g/g lignin consumed	-	-	0.93	-	0.93	-	0.93	-	1.19	0.93
Overall carbon upgrading efficiency to coproduct ^d	mol %	-	-	4.0%	-	4.0%	-	4.0%	-	5.4%	30.1%
Fermentation productivity	g/L/h	-	-	0.06 (0.53)	-	0.06 (0.53)	-	0.06 (0.53)	-	0.23	1
Coproduct production	MMlb/yr	-	-	30	-	31	-	29	-	35	187

^a 2018–2020 lignin conversion "base" case from actual black liquor/BCD hydrolysate; "high" case (in parentheses) = highest productivity observed to date based on model lignin monomers. 2021 lignin conversion to BKA only reflected actual hydrolysate (akin to "base" case previously).

^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.

[°] First number represents sugar conversion to desired product (BDO/acids); values in brackets indicate total sugar utilization (including biomass organism propagation).

^d Includes fermentation of all convertible components, plus product recovery and subsequent upgrading (adipic acid cases)

^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 lignin coproduct.

Table 2 and Figure 2 also show the detailed comparisons between the 2021 SOT scenarios, the 2017–2020 back-cast SOTs, 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 toward 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. With the new two-stage DMR pretreatment approach maintained here, biomass deconstruction yields through enzymatic hydrolysis are nearly at their targets for the batch hydrolysis approach (now exceeding the target for xylan conversion and nearly at the target for glucan conversion, at 88% SOT vs. 90% targeted using 10 mg/g enzyme loading). Still, further room for improvement exists regarding development of enzymes more tailored to DMR pretreatment, which will require not only more fundamental understanding of biomass recalcitrance, but also continuous collaborations and efforts between national labs 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 2021 SOT benchmarks. In the BDO pathway, fermentation yields have already nearly achieved final 2030 goals (on whole-slurry hydrolysate), with the exception of arabinose utilization, which must be engineered into the organism, while also nearly doubling the fermentation productivity. However, identifying ways to increase BDO titers will also be of important significance to further reduce MFSPs, either through new fermentation strategies (e.g., hydrolysate clarification and fed-batch fermentation) or through non-distillation BDO concentration strategies (as being investigated under the Separations Consortium). Another 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.

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-h targets vs. 0.6-g/L-h 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 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 continues to remain in the lignin-to-coproducts train. As noted above and consistent with prior SOTs, despite the high value

of the coproduct (adipic acid or BKA), the current experimental benchmark data translate to a higher cost to produce the product than the coproduct revenues it generates, driven most strongly by low bioconversion productivity (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). However, overall process yields to BKA have been improved by 17% while also improving fermentation productivity roughly fourfold over prior muconic/adipic acid benchmarks. Still, relative to 2021 SOT levels, the lignin train must improve by 2030 to achieve a further fourfold improvement in productivity (from 0.23 up to 1.0 g/L-h) and eightfold improvement in overall lignin conversion (from 0.19 to 1.6 g/g soluble lignin process yields) in order to improve overall coproduct outputs from 34 to roughly 190 million pounds per year in the modeled biorefinery. This continues to highlight that lignin deconstruction/upgrading generally represents the largest-risk area of the integrated process in ultimately achieving future MFSP goals. As such, currently and moving forward, the Biochemical Analysis project continues to place a primary focus around evaluating potential alternative "contingency strategies" in collaboration with NREL research projects that also may enable MFSP reductions through other processing approaches (based on experimental efforts being undertaken in such areas).

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



Figure 2(a). Tracking SOT progression from 2017–2021, compared to out-year 2030 projection (BDO pathway)



Figure 2(b). Tracking SOT progression from 2017–2021, compared to out-year 2030 projection (acids pathway)

Sustainability Metric Indicators

In addition to the TEA results noted above, we also report here on associated sustainability "indicators" attributed to the SOT conversion model scenarios. In keeping with recent Bioenergy Technologies Office 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 the Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies [GREET] model 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.

The BDO pathway reflects a small increase in mass/carbon yield to fuels for the 2021 SOT case relative to 2020 attributed to improved BDO upgrading and oligomerization yields, while the acids pathway maintains the same values for these metrics as the prior SOT. Both pathways also require a net power import in all cases evaluated due to power demands throughout the facility (driven by mechanical refining pretreatment, mechanical vapor recompression sugar evaporation, where relevant, and aerobic lignin bioconversion power demands), as well as heat demands diverting steam away from the steam turbine generators. With the switch to lignin conversion to BKA rather than muconic/adipic acid, natural gas demands have increased in the present SOT relative to prior levels due to higher energy requirements for BKA product recovery/purification. Water consumption per GGE fuel decreased for the lignin conversion cases in 2021 following trends in fuel yield improvements, though increased for the lignin conversion cases, again attributed to the new operations employed for BKA coproduct recovery.

 Table 3. Sustainability Indicators for 2017–2021 SOT and Future Projection Scenario

	2017 SOT (Burn Lignin)	2018 SOT (Burn Lignin)	2018 SOT Convert Lignin: Base (High)	2019 SOT (Burn Lignin)	2019 SOT Convert Lignin: Base (High)	2020 SOT (Burn Lignin)	2020 SOT Convert Lignin: Base (High)	2021 SOT (Burn Lignin)	2021 SOT Convert Lignin: BKA	2030 Projection (Convert Lignin)
BDC) Pathway	-		-	-	-				
Fuel yield by weight of biomass (wt % of dry biomass)	9.6%	9.9%	9.9%	11.7%	11.7%	12.6%	12.7%	13.0%	13.1%	13.2%
Carbon efficiency to fuels (% feedstock C)	18.2%	18.7%	18.7%	22.1%	22.1%	23.8%	23.9%	24.5%	24.6%	25.0%
Carbon efficiency to lignin coproduct (% feedstock C)	NA	NA	2.3%	NA	2.3%	NA	2.2%	NA	2.4%	14.8%
Net electricity import (kWh/GGE)	12.3	5.1	14.0	5.7	12.5 (12.6)	4.9	11.4 (11.5)	6.3	10.6	10.5
Net natural gas import (Btu/GGE [LHV]ª)	0	0	75,284 (76,789)	0	69,928	0	60,607	0	85,593	14,596
Water consumption (gal water/GGE)	23.4	13.9	11.3 (11.5)	10.9	9.2	9.3	7.8	8.0	10.1	8.9
Acio	ls Pathwa	y		-	-	-				
Fuel yield by weight of biomass (wt % of dry biomass)	8.1%	8.6%	8.6%	10.8%	10.8%	11.8%	11.8%	11.8%	11.8%	13.8%
Carbon efficiency to fuels (% feedstock C)	15.5%	16.3%	16.3%	20.6%	20.6%	22.5%	22.4%	22.5%	22.4%	26.2%
Carbon efficiency to lignin coproduct (% feedstock C)	NA	NA	2.3%	NA	2.3%	NA	2.2%	NA	2.4%	14.4%
Net electricity import (kWh/GGE)	5.8	1.3	21.5 (21.6)	2.8	17.4 (17.6)	2.2	15.5 (15.6)	2.2	16.4	10.7
Net natural gas import (Btu/GGE [LHV])	0	15,790	15,790	11,803	11,803	11,064	11,035	11,064	12,528	9,055
Water consumption (gal water/GGE)	30.7	36.0	26.0 (26.1)	27.7	20.0	24.7	17.9	24.7	19.7	13.5

^a Lower heating value

Concluding Remarks

The work presented here provides a re-benchmarking of NREL's Biochemical Platform efforts in moving toward future design case goals. Based on data availability for 2021 experimental work on integrated hydrolysate processing, the 2021 SOT considers two bioconversion pathways for hydrocarbon fuel production, namely BDO and carboxylic acids. Biomass deconstruction efforts maintain prior performance at 88% glucan conversion, >93% xylan conversion, and 91% arabinan conversion to monomeric sugars through saccharification at 10-mg/g total enzyme loading, enabled by a recent two-stage DMR pretreatment approach employed in 2020 making use of sodium carbonate to reduce more costly sodium hydroxide usage (also yielding notable LCA improvements). Sugar fermentation performance was not seen to improve over 2020 levels, and thus 2020 SOT benchmarks were maintained for those operations, although those prior data were already 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). Catalytic upgrading performance for the BDO fuel pathway was improved over 2020 levels with better yields/selectivities and kinetics (space velocity), while catalysis parameters were maintained at 2020 levels for the acids pathway. The resulting 2021 SOT benchmark MFSPs are estimated to be \$6.62/GGE and \$7.07/GGE (\$4.79/GGE and \$5.04/GGE conversion-only costs excluding feedstock contributions at \$78/ton) in 2016 dollars based on combustion of all lignin and residual solids for the BDO and acids pathways, respectively. Relative to the previous 2020 SOT basis, this translates to an improvement of \$0.18/GGE and \$0.05/GGE in overall MFSPs for the two respective pathways.

The primary area for cost reduction in this year's SOT was associated with lignin conversion to coproducts, with 2021 SOT MFSP estimates of **\$8.65/GGE and \$9.33/GGE for lignin conversion** performance on biomass hydrolysate (BDO and acids pathways, respectively). These results maintain that the lignin-to-coproduct train is not yet economically profitable relative to burning the lignin, given higher costs for producing the coproduct than the amount of coproduct revenue generated (attributed in turn to low lignin deconstruction/conversion yields and fermentation productivities observed to date). However, performance parameters for the lignin coproduct train were considerably improved, owing to a shift in focus from two-stage muconic/adipic acid production to single-stage BKA production, with higher BKA yields and productivities combined with lower process complexity enabling MFSP reductions of roughly \$0.7–\$0.8/GGE relative to 2020 SOT benchmarks for adipic acid coproduction. If BKA market prices could fetch a premium over adipic acid given BKA's property/performance advantages, these MFSPs could be reduced by roughly \$0.10–\$0.20/GGE for a price premium of 10% and 20%, respectively.

Analysis of sustainability metric indicators from the Aspen SOT conversion models demonstrates BDO fuel yields of 13.0% by weight or 24.5% by carbon retention relative to biomass feedstock, along with 2.4% carbon yields to BKA coproduct in the "convert lignin" scenarios. Fuel yields are slightly lower for the acids case at 11.8% by weight or 22.5% by carbon utilization, with the same 2.4% carbon yield basis to BKA. Net power imports are calculated as 6.3 kWh/GGE for the BDO case or 2.2 kWh/GGE for the acids case in the "burn lignin" scenario, increasing to 10.6 and 16.4 kWh/GGE, respectively, in the "convert lignin" scenario (due to substantial power demands for aerobic lignin bioconversion at low fermentation productivities). Approximately 86,000 Btu/GGE of supplemental natural gas is required for the 2021 SOT BDO cases including lignin conversion, but none is required for the "burn lignin" scenario, while for the acids case, roughly 11,000 Btu/GGE of natural gas is required for the "burn lignin" 2021 SOT case, increasing to roughly 13,000 BTU/GGE for the "convert lignin" scenario. Finally, water consumption is estimated at 8.0 gal/GGE for the BDO "burn lignin" case, and roughly 10.1 gal/GGE for the BDO "convert lignin" case. Water consumption is higher at 24.7 gal/GGE in the acids "burn lignin" case, reducing to 19.7 gal/GGE 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, the deacetylation step may be further optimized by increasing liquor concentrations and reducing carbohydrate losses into the soluble liquor fraction (e.g., through continuous counter-current alkaline extraction rather than batch deacetylation). 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 already beginning to approach or in some cases exceed final targets). A key operation undergoing continued R&D focus and optimization in the Separations Consortium for the acids pathway is around low-cost recovery of the intermediate acids utilizing continuous pertraction at high recovery efficiencies (including better understanding scale-up implications on design and cost details) or alternative approaches to avoid significant fresh caustic/acid demands-or, most ideally, achieving low-pH fermentation without the need for any acids isolation operations. Finally, further and more significant improvements are required in the lignin coproduct train in order to first break even and ultimately lower MFSPs toward 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 beyond the latest improvements achieved in the past year.

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Appendix A. TEA Summary Sheets for 2021 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\$

\$6.62 /GGE

\$1.83 /GGE

\$4.79 /GGE

\$0.00 /GGE

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent

Basis):

Contributions: Feedstock Fuel Conversion Coproduct Conversion

Fuel Production Fuel Yield BKA Coproduct Yield 2,3-Butanediol Process Yield [Theoretical Yield] Feedstock + Handling Cost Internal Rate of Return (After-Tax) Equity Percent of Total Investment

30.9	MMGGE per year (at 68 °F)
42.7	GGE / dry U.S. ton feedstock
0	lb / dry U.S. ton feedstock
0.45	[0.5] kg BDO/kg Total Sugars (89% of theoretical)
\$78.21	/dry U.S. ton feedstock
10%	
40%	

Capital Costs			
Area 200: Pretreatment	\$51,445,817		
Area 300: Sugar Hydrolysis and Conditioning	\$26,249,893		
Area 400: Enzyme Production	\$11,520,765		
Area 500: Bioconversion and Upgrading	\$72,329,857		
Area 600: Wastewater	\$56,152,044		
Area 700: Lignin	\$0		
Area 800: Boiler	\$65,462,371		
Area 900: Utilities & Storage	\$11,897,439		
	4005 050 105		
Total Installed Equipment Cost	\$295,058,185		
Added Direct + Indirect Costs	\$249,941,815		
(% of TCI)	46%		
Total Capital Investment (TCI)	\$545,000,000		
Installed Equipment Cost/Annual GGE	\$9.53		
Total Capital Investment/Annual GGE	\$17.61		
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)	47.9%		
From Biomass (Fuel C / Biomass C)	24.5%		
BKA 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	94,315		
Current Yield (Actual/Theoretical)	62.4%		

^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 produc	:t)
Feedstock + Handling	183.1
Sulfuric Acid	0.0
Caustic	26.8
Sodium Carbonate	31.9
Glucose (enzyme production)	27.0
Hydrogen	35.6
Electricity (import)	41.3
Other Raw Materials	71.4
Catalysts	8.9
Waste Disposal	4.6
Na2SO4 Coproduct	-42.0
BKA coproduct (\$0.86/lb)	0.0
Fixed Costs	47.1
Capital Depreciation	55.6
Average Income Tax	17.2
Average Return on Investment	153.3
Total	661.8
Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$56,700,000
Sulfuric Acid	\$0
Caustic	\$8,300,000
Glucose (enzyme production)	\$8,400,000
Hydrogen	\$11,000,000
Electricity (import)	\$12,800,000
Other Raw Materials	\$22,100,000
Catalysts	\$2,700,000
Waste Disposal	\$1,400,000
Na2SO4 Coproduct	-\$13,000,000
BKA coproduct (\$0.86/lb)	\$0
Fixed Costs	\$14,600,000
Capital Depreciation	\$17,200,000
	\$5,200,000
Average Boturn on Investment	\$3,300,000
Total	\$47,400,000
Total	\$194,900,000
Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	6.3
Plant Electricity Lise (kWh/GGE)	12.6
Metabolic Yield (a/a substrate)	12.0
Glucose to 2.3_BDO	0.482
Glucose to Biomass	0.402
VIII 10000000000000000000000000000000000	0.030

0.481

0.027

0.000

0.820

Xylose to 2,3-BDO

Xylose to Biomass

Arabinose to 2,3-BDO

Arabinose to Biomass

BDO Pathway (Convert Lignin – BKA)

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):

Feedstock Contributions: Fuel Conversion Coproduct Conversion

65.12 /GGE \$1.70 /GGE

Fuel Production Fuel Yield BKA Coproduct Yield 2,3-Butanediol Process Yield [Theoretical Yield] Feedstock + Handling Cost Internal Rate of Return (After-Tax) Equity Percent of Total Investment

\$1.82	/GGE
\$5.12	ICCE

\$8.65 /GGE

31.0 MMGGE per year (at 68 °F) 42.9 GGE / dry U.S. ton feedstock 47 lb / dry U.S. ton feedstock 0.45 [0.5] kg BDO/kg Total Sugars (89% of theoretical) \$78.21 /dry U.S. ton feedstock 10% 40%

Capital Costs	
Area 200: Pretreatment	\$51,390,153
Area 300: Sugar Hydrolysis and Conditioning	\$26,249,944
Area 400: Enzyme Production	\$11,520,765
Area 500: Bioconversion and Upgrading	\$72,353,170
Area 600: Wastewater	\$56,237,036
Area 700: Lignin	\$226,470,064
Area 800: Boiler	\$54,416,455
Area 900: Utilities & Storage	\$13,175,918
Total Installed Equipment Cost	\$511,813,504
Added Direct + Indirect Costs	\$463,986,496
(% of TCI)	48%
Total Capital Investment (TCI)	\$975,800,000
Installed Equipment Cost/Annual GGE	\$16.49
Total Capital Investment/Annual GGE	\$31.43
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)	48.1%
From Biomass (Fuel C / Biomass C)	24.6%
BKA Carbon Efficiency from Biomass	2.4%
Maximum Yields (100% of Theoretical) ^a	
Fuel Production (U.S. ton/yr)	151,073
Current Fuel Production (U.S. ton/yr) ^b	94,587
Current Yield (Actual/Theoretical)	62.6%

^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	182.5
Sulfuric Acid	25.3
Caustic	47.8
Sodium Carbonate	31.8
Glucose (enzyme production)	27.0
Hydrogen	35.4
Electricity (import)	71.1
Other Raw Materials	99.5
Catalysts	9.5
Waste Disposal	4.7
Na2SO4 Coproduct	-54.6
BKA coproduct (\$0.86/lb)	-94.3
Fixed Costs	78.1
Capital Depreciation	99.5
Average Income Tax	30.1
Average Return on Investment	271.4
Total	864.9
Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$56,700,000
Sulfuric Acid	\$7,900,000
Caustic	\$14,800,000
Glucose (enzyme production)	\$8,400,000
Hydrogen	\$11,000,000
Electricity (import)	\$22,100,000
Other Raw Materials	\$30,900,000
Catalysts	\$2,900,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$17,000,000
BKA coproduct (\$0.86/lb)	-\$29,300,000
Fixed Costs	\$24,200,000
Capital Depreciation	\$30,900,000
Average Income Tax	\$9,300,000
Average Return on Investment	\$84,300,000
Total	\$258,600,000
Specific Operating Conditions	

Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	10.6
Plant Electricity Use (kWh/GGE)	13.5
Metabolic Yield (g/g substrate)	
Glucose to 2,3-BDO	0.482
Glucose to Biomass	0.030
Xylose to 2,3-BDO	0.481
Xylose to Biomass	0.027
Arabinose to 2,3-BDO	0.000
Arabinose to Biomass	0.818

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):

Contributions: Feedstock Fuel Conversion Coproduct Conversion

\$7.07 /GGE \$2.03 /GGE \$5.04 /GGE

\$0.00 /GGE

Fuel Production Fuel Yield BKA Coproduct Yield Butyric Acid Process Yield [Theoretical Yield] Feedstock + Handling Cost Internal Rate of Return (After-Tax) Equity Percent of Total Investment

Capital Costs			
Area 200: Pretreatment	\$51,445,817		
Area 300: Sugar Hydrolysis and Conditioning	\$82,903,853		
Area 400: Enzyme Production	\$11,520,765		
Area 500: Bioconversion and Upgrading	\$49,013,154		
Area 600: Wastewater	\$60,270,174		
Area 700: Lignin	\$0		
Area 800: Boiler	\$69,608,234		
Area 900: Utilities & Storage	\$11,776,742		
Total Installed Equipment Cost	\$336,538,739		
Added Direct + Indirect Costs	\$287.961.261		
(% of TCI)	46%		
Total Capital Investment (TCI)	\$624,500,000		
Installed Equipment Cost/Annual GGE	\$12.08		
Total Capital Investment/Annual GGE	\$22.41		
Operating Hours Per Year (On-Stream Factor)	7884 (90%)		
Loan Rate	8.0%		
Term (years) Capital Charge Factor (Computed)	10 0 127		
Fuel Carbon Retention Efficiencies:	10.00/		
From Hydrolysate Sugar (Fuel C / Sugar C)	46.2%		
From Biomass (Fuel C / Biomass C)	22.5%		
BKA Carbon Enciency 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	85,467		
Current Yield (Actual/Theoretical)	66.4%		

^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) 27.9 MMGGE per year (at 68 °F)
38.5 GGE / dry U.S. ton feedstock
0 lb / dry U.S. ton feedstock
0.44 [0.49] kg Acid/kg Total Sugars (89% of theoretical)
\$78.10 /dry U.S. ton feedstock
10%
40%

Manufacturing Costs (cents/GGE fuel product)

Feedstock + Handling	203.0
Sulfuric Acid	0.0
Caustic	29.7
Sodium Carbonate	35.5
Glucose (enzyme production)	30.0
Hydrogen	0.0
Electricity (import)	13.5
Other Raw Materials	90.3
Catalysts	2.3
Waste Disposal	5.1
Na2SO4 Coproduct	-45.4
BKA coproduct (\$0.86/lb)	0.0
Fixed Costs	57.8
Capital Depreciation	71.1
Average Income Tax	21.6
Average Return on Investment	192.8
Total	707.4
Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$56,600,000
Sulfuric Acid	\$0
Caustic	\$8,300,000
Glucose (enzyme production)	\$8,400,000
Hydrogen	\$0
Electricity (import)	\$3,800,000
Other Raw Materials	\$25,200,000
Catalysts	\$600,000
Waste Disposal	\$1,400,000
Na2SO4 Coproduct	-\$12,700,000
BKA coproduct (\$0.86/lb)	\$0
Fixed Costs	\$16,100,000
Capital Depreciation	\$19,800,000
Average Income Tax	\$6,000,000
Average Return on Investment	\$53,700,000
Total	\$187,200,000
Specific Operating Conditions	
operating operating containents	

Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	2.2
Plant Electricity Use (kWh/GGE)	15.7
Metabolic Yield (g/g substrate)	
Glucose to Butyric	0.46
Glucose to Biomass	0.02
Xylose to Butyric	0.46
Xylose to Biomass	0.02
Arabinose to Butyric	0.14
Arabinose to Biomass	0.02

Acids Pathway (Convert Lignin – BKA)

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):

Contributions: Feedstock Fuel Conversion Coproduct Conversion \$2.04 /GGE \$5.26 /GGE

\$9.33 /GGE

Fuel Production Fuel Yield BKA Coproduct Yield Butyric Acid Process Yield [Theoretical Yield] Feedstock + Handling Cost Internal Rate of Return (After-Tax) Equity Percent of Total Investment

Capital Costs			
Area 200: Pretreatment	\$51,445,817		
Area 300: Sugar Hydrolysis and Conditioning	\$82,903,853		
Area 400: Enzyme Production	\$11,520,765		
Area 500: Bioconversion and Upgrading	\$49,002,750		
Area 600: Wastewater	\$54,777,391		
Area 700: Lignin	\$225,821,769		
Area 800: Boiler	\$32,293,458		
Area 900: Utilities & Storage	\$12,240,617		
Total Installed Equipment Cost	\$520,006,420		
Added Direct + Indirect Costs	\$479,093,580		
(% of TCI)	48%		
Total Capital Investment (TCI)	\$999,100,000		
Installed Equipment Cost/Annual GGE	\$18.70		
Total Capital Investment/Annual GGE	\$35.93		
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)	46.1%		
From Biomass (Fuel C / Biomass C)	22.4%		
BKA Carbon Efficiency from Biomass	2.4%		
Maximum Yields (100% of Theoretical) ^a			
Fuel Production (U.S. ton/yr)	128,798		
Current Fuel Production (U.S. ton/yr) ^b	85,310		
Current Yield (Actual/Theoretical)	66.2%		

^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) \$2.03 /GGE
27.8 MMGGE per year (at 68 °F)
38.4 GGE / dry U.S. ton feedstock
48 lb / dry U.S. ton feedstock
0.44 [0.49] kg Acid/kg Total Sugars (89% of theoretical)
\$78.21 /dry U.S. ton feedstock
10%

40%

Manufacturing Costs (cents/GGE fuel product)

Feedstock + Handling	203.7
Sulfuric Acid	30.6
Caustic	63.8
Sodium Carbonate	35.55
Glucose (enzyme production)	30.1
Hydrogen	0.0
Electricity (import)	110.0
Other Raw Materials	74.0
Catalysts	3.1
Waste Disposal	5.3
Na2SO4 Coproduct	-64.6
BKA coproduct (\$0.86/lb)	-106.5
Fixed Costs	91.2
Capital Depreciation	114.0
Average Income Tax	34.1
Average Return on Investment	309.0
Total	933.2
Manufacturing Costs (\$/yr)	
Feedstock + Handling	\$56,700,000
Sulfuric Acid	\$8,500,000
Caustic	\$17,700,000
Glucose (enzyme production)	\$8,400,000
Hydrogen	\$0
Electricity (import)	\$30,600,000
Other Raw Materials	\$20,600,000
Catalysts	\$900,000
Waste Disposal	\$1,500,000
Na2SO4 Coproduct	-\$18,000,000
BKA coproduct (\$0.86/lb)	-\$29,600,000
Fixed Costs	\$25,400,000
Capital Depreciation	\$31,700,000
Average Income Tax	\$9,500,000
Average Return on Investment	\$85,900,000
Total	\$249,800,000
Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	16.4
Plant Electricity Use (kWh/GGE)	18.2
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
Arabinose to Butyric	0.108
Arabinose to Biomass	0.074

Appendix B. Life Cycle Inventory (LCI) for 2021 SOT Benchmark Models

BDO Pathway

	2021 SOT (Burn Lignin)	2021 SOT (Convert	
		Lignin – BKA)	<u>.</u>
Products	Production Rate)	
Hydrocarbon fuel	10,851	10,882	kg/h
	115	115	MM kcal/h (LHV)
Coproducts			
Beta-ketoadipate	0	1,968	kg/h
Recovered sodium sulfate salt from WWT	10,581	13,810	kg/h
Export electricity	-	-	kW
Resource Consumption	Flow Rate (kg/h)		
Biomass feedstock (20% moisture)	104,167	104,167	
Sulfuric acid, 93%	9,235	10,521	
Caustic (as pure)	2,000	3,582	
Sodium carbonate	6,667	6,667	
Ammonia	1,160	2,189	
Glucose	1,312	1,312	
Corn steep liquor	918	918	
Corn oil	7	7	
Host nutrients	37	37	
Sulfur dioxide	9	9	
Diammonium phosphate	103	103	
Flocculant	435	436	
Toluene solvent makeup	0	0	
Hydrogen	868	865	
Ethanol	0	0	
Boiler chemicals	0	1	
Flue gas desulfurization lime	109	183	
WWT polymer	34	0	
Cooling tower chemicals	2	1	
Makeup water	119,427	150,469	
Natural gas for boiler	0	6,400	
Natural gas for hot oil system	0	0	MMBtu/h
Grid electricity (net import)	23,768	41,073	kW
Waste Streams	Flow Rate (kg/h)		
Disposal of ash	4,290	4,414	<u>.</u>
Air Emissions	Flow Rate (kg/h)		
H ₂ O	96,144	101,016	
N ₂	508,785	426,513	
CO ₂	108,250	121,885	
O ₂	80,408	29,481	
NO ₂	23	36	
SO ₂	7	12	
CO	81	66	
CH ₄	3	0	

2021 SOT 2021 SOT (Convert (Burn Lignin) Lignin – BKA) **Products Production Rate** Hydrocarbon fuel 9.833 9,815 kg/h MM kcal/h (LHV) 103 103 Coproducts Beta-ketoadipate 0 1,991 kg/h Recovered sodium sulfate salt from WWT 10,304 14,639 kg/h Export electricity kW -Flow Rate (kg/h) **Resource Consumption** 104,167 Biomass feedstock (20% moisture) 104,167 11,375 Sulfuric acid, 93% 9,235 Caustic (as pure) 4,280 2,000 Sodium carbonate 6,667 6.667 Ammonia 1,261 2.319 Glucose 1,312 1,312 Corn steep liquor 1,226 1,226 Corn oil 7 7 Host nutrients 37 37 9 9 Sulfur dioxide Diammonium phosphate 169 169 Flocculant 407 407 Toluene solvent makeup 90 90 Hydrogen 0 0 Ethanol 0 0 **Boiler chemicals** 0 0 Flue gas desulfurization lime 111 197 WWT polymer 37 0 Cooling tower chemicals 3 1 Makeup water 330,952 262,876 Natural gas for boiler 0 100 39 MMBtu/h Natural gas for hot oil system 39 Grid electricity (net import) 7,019 56,869 kW Waste Streams Flow Rate (kg/h) 4,294 Disposal of ash 4,437 **Air Emissions** Flow Rate (kg/h) H₂O 125,107 91,211 N₂ 485,922 598,415 CO_2 112,524 109,747 75,224 111,143 **O**₂ NO₂ 47 6 SO₂ 8 12 CO 83 30

Acids Pathway

CH₄

2

0