Biochemical Conversion of Lignocellulosic Biomass to Hydrocarbon Fuels and Products: 2022 State of Technology and Future Research

Ryan Davis and Andrew Bartling

National Renewable Energy Laboratory

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NOTICE

Acknowledgments

List of Acronyms

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
ETJ	ethanol-to-jet
GGE	gallon gasoline equivalent
GHG	greenhouse gas
INL	Idaho National Laboratory
IS	insoluble solids
ISPR	*in situ* product recovery
LCA	life cycle analysis
LHV	lower heating value
MEK	methyl ethyl ketone
MFSP	minimum fuel selling price
NREL	National Renewable Energy Laboratory
ORNL	Oak Ridge National Laboratory
RCF	reductive catalytic fractionation
SAF	sustainable aviation fuel
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 a key 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 biofuel technology.

Building upon efforts to progress 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.

Building on recent improvements in lignin valorization initially reflected in 2021, experimental efforts in lignin upgrading over the past year continued to optimize work on production of β-ketoadipate (BKA) as a more optimal molecule compared to the closely related adipic acid coproduct of prior 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 production of BKA). 2022 SOT performance achieved a substantial threefold improvement in BKA fermentation productivity and 33% increase in yield compared to 2021 SOT benchmarks, with yields well exceeding theoretical based on available lignin monomers, implying utilization of additional carbon likely from lignin oligomers.

Beyond lignin upgrading to coproducts, additional improvements were made through further optimization of deacetylation and mechanical refining pretreatment utilizing two-stage alkali extraction to reduce sodium hydroxide usage while increasing sugar yields, as well as employing a new BDO fermentation strain capable of utilizing arabinose sugars. Altogether, these modifications translated to very favorable sugar yields from enzymatic hydrolysis at 89% glucan conversion, 94% xylan conversion, and 70% arabinan conversion to monomeric sugars at 10-mg/g enzyme loading, coupled with nearly 100% conversion of all three available sugars to theoretical yields across BDO fermentation. Carboxylic acid platform efforts primarily focused upon bioprocess integration and scale-up, as well as downstream separations improvements, which improved process robustness but not direct fermentation metrics; thus, prior SOT benchmarks were maintained though also have already largely met future 2030 targets at 95% conversion of glucose and xylose to acid fermentation products. Catalytic upgrading metrics

remained largely unchanged for both pathways, with the exception of recent experimental findings in the acid pathway indicating a more realistic weight hourly space velocity of 0.4 h^{-1} required to maintain catalyst activity for the ketonization step rather than 4.0 h^{-1} as previously asserted.

Based on the combination of these process parameter values, the 2022 SOT MFSPs are estimated to be $6.24/GGE and $7.02/GGE ($4.58/GGE and $5.06/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 47.1 and 40.0 GGE/ton dry biomass for the respective pathways. These results translate to a reduction of $0.38/GGE and $0.05/GGE in overall MFSPs for the two respective pathways relative to the 2021 SOT. The 2022 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.

Alternatively, the SOT scenarios reflecting lignin conversion to coproducts indicated MFSP estimates of $7.60/GGE and $8.61/GGE for experimental lignin conversion performance on biomass hydrolysate (BDO and acids pathways, respectively). This represents a $1.05 and $0.72/GGE reduction, respectively, relative to 2021 SOT benchmarks, attributed to enhancements in BKA coproduct conversion rate and yield from bioconversion of lignin components noted earlier, with a sensitivity case indicating that a further $0.12–$0.28/GGE reduction would be incurred if BKA could fetch a price premium over adipic acid of 10%–20%, respectively. Though substantial progress has been made in the lignin conversion process as shown by these MFSP improvements, 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 primarily to low lignin deconstruction yields under the current framework via base-catalyzed deconstruction). This again highlights lignin processing as a key priority moving forward for future focus in ultimately contributing to 2030 MFSP viability goals.

This report also documents 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). Finally, in light of increased prioritization by the U.S. Department of Energy's Bioenergy Technologies Office (BETO) toward deeper decarbonization, maximizing sustainable aviation fuel, and emphasizing near-term technology deployment potential, opportunities for modifying the current SOT pathways as well as pursuing new pathway configurations are presented as candidates for future consideration moving forward.

Table ES-1. Summary of MFSPs and Fuel Yields for 2022 SOT Cases Compared to 2017–2021 SOT[a]

	BDO 2017 SOT Burn Lignin	Acids 2017 SOT Burn Lignin	BDO 2018 SOT Burn (Convert)	Acids 2018 SOT Burn (Convert)	BDO 2019 SOT Burn (Convert)	Acids 2019 SOT Burn (Convert)	BDO 2020 SOT Burn (Convert)	Acids 2020 SOT Burn (Convert)	BDO 2021 SOT Burn (Convert)	Acids 2021 SOT Burn (Convert)	BDO 2022 SOT Burn (Convert)	Acids 2022 SOT Burn (Convert)
MFSP ($/GGE, 2016$)	$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)	$6.24 ($7.60)	$7.02 ($8.61)
Feedstock contribution ($/GGE, 2016$)	$2.67	$3.19	$2.59	$2.99	$2.11	$2.30	$1.93	$2.09	$1.83	$2.03	$1.66	$1.95
Conversion contribution ($/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)	$4.58 ($5.93)	$5.06 ($6.65)
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	47.1	40.0

[a] 2018–2022 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 "n^{th}-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 whole-slurry 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 2022 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 MFSP 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 (based on historical program goals developed previously), 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, application/use and associated costs of commercial enzymes, etc. 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 a newer, more novel 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 in the target design cases given significantly lower chemical oxygen demand (COD) levels than prior designs. Both pathways also assume on-site enzyme production following a consistent framework for this operation as applied in past historical SOTs (due to unavailable information on commercially purchased enzyme costs at scale, though recognizing the latter would be the likely approach taken in a commercial biorefinery today). Finally, residual solids, wastewater sludge, and off-gas streams are combusted in a boiler connected to a steam turbine generator set to provide combined heat and power benefits to the facility.

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

1. DMR step – deacetylation/alkaline extraction: While the future target asserts the use 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 SOTs. However, a key update in recent SOTs 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). The latest SOT refinements reflect strain development for arabinose use with near-100% utilization exceeding design case targets.

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 2019–2022 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 moved to a new, though closely related molecule of interest, based on β-ketoadipate (BKA) rather than adipic acid as the focus for lignin coproduct valorization – the BKA approach is maintained in the 2022 SOT with further improvements over the 2021 benchmarks documented here. 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 historical SOTs

      i. 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.
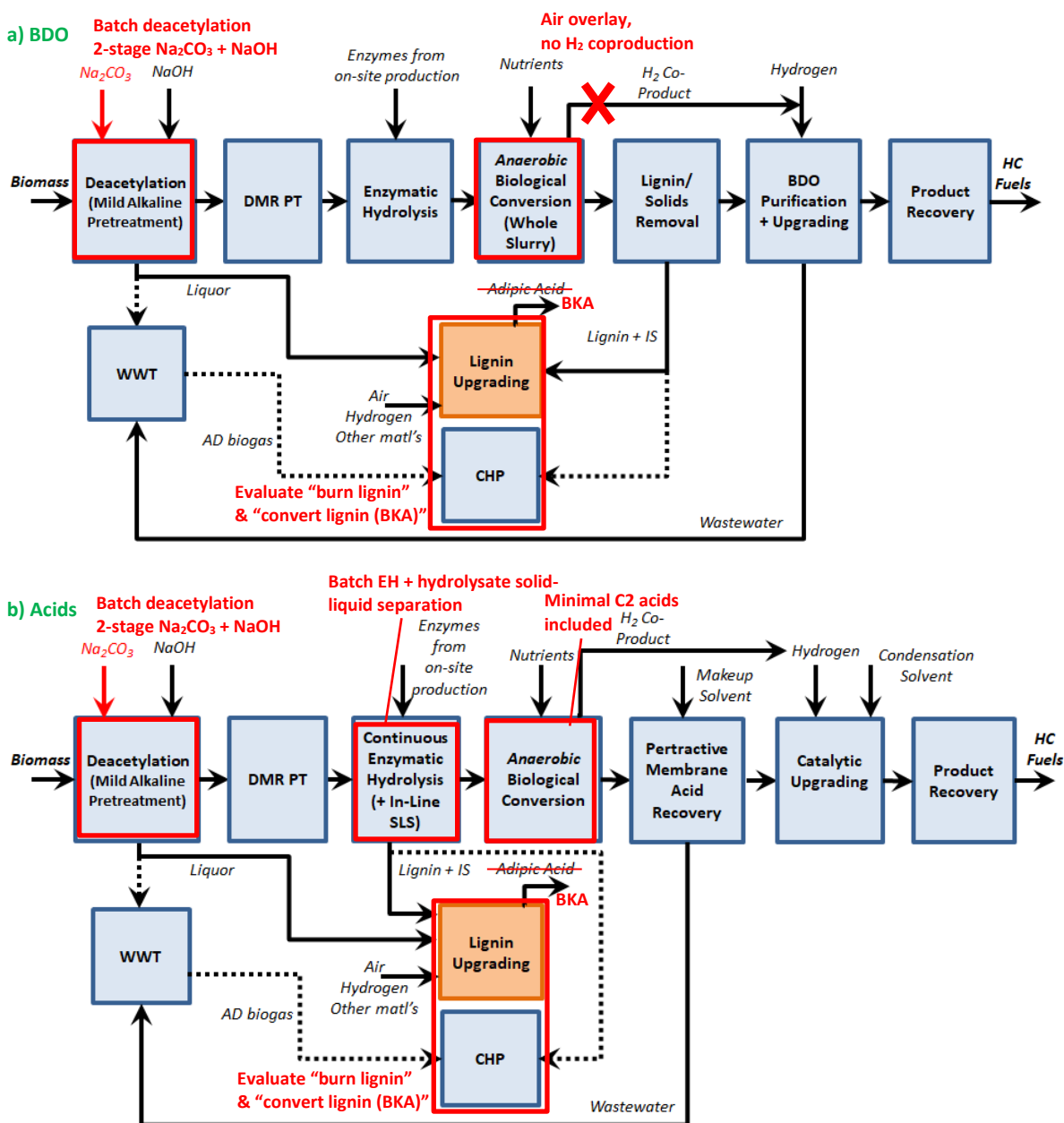
Figure 1. Block diagram schematics for 2030 "advanced process" configurations as projected in the 2018 design report [2]. Modifications from the 2030 goals as reflected in the current 2022 SOT are denoted in red.

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Feedstock

Consistent with prior years, feedstock assumptions for the SOT between 2017 and 2022 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 2022 SOT, INL moved to a new approach for corn stover feedstock logistics, based on adding an air classification step to fractionate the corn stover into its constituent anatomical fractions (cobs, husks, stalks, and leaves) based on encouraging preliminary findings for this approach identified under the Feedstock-Conversion Interface Consortium (FCIC) [5] . Under that approach, fractionated tissues may either be processed separately through staged biorefinery conversion campaigns tailoring each step's operating conditions as optimal for each individual fraction, or may be recombined under different ratios to meet compositional quality specifications (for example by removing some or all of one fraction). For SOT purposes, the latter approach is assumed here based on running a blend of fractionated tissues at a constant blend ratio across the year that achieves the SOT compositional targets (consistent with prior SOTs which also have been based on various blends of two-pass and three-pass stover and/or other herbaceous biomass feedstocks). The fractionated leaves contain a higher ash content than the other fractions, and are diverted and sold as a coproduct to be blended into agricultural feed markets. The resulting blended material achieves a consistent delivered feedstock cost as the prior year's SOT at $78.21/ton while reducing ash dockage costs and meeting or exceeding the 59% carbohydrate specification, though lower feedstock costs could be achieved at higher coproduct values for diverting and selling the leaves fraction (personal communication with David Thompson/Damon Hartley, INL, September 2022).

Table 1. Feedstock Costs Adjusted to 5% Ash for Years 2017–2022 (2016-year dollars; courtesy of David Thompson, Damon Hartley, and Mohammad Roni, INL)

	2017	2018	2019	2020	2021	2022
Total feedstock cost to biorefinery at 5% ash equivalent ($/dry ton)	$83.90	$83.67	$81.37	$80.10	$78.21	$78.21
Ash dockage vs. 5% baseline ($/dry ton) [a]	$1.26	$1.24	$1.58	$1.39	$0.38	$0.01

[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. 2022).

Pretreatment and Enzymatic Hydrolysis

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 generally 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 (although alternative lignin fractionation approaches are also possible). 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 [6], 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 2017–2021 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 [7]. 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 [8]. Accordingly, in 2020, NREL's Low-Temperature Advanced Deconstruction project focused research efforts on a two-stage deacetylation approach making use of sodium carbonate (Na_2CO_3) 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 [9], with an optimal case identified at a Na_2CO_3 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. Further experimental work was conducted on this concept in support of the 2022 SOT, and found slightly better yield performance based on loadings of 90 and 33 kg/dry tonne for Na_2CO_3 and NaOH respectively, which was found to maximize GHG reduction benefits compared to three other two-stage scenarios or the NaOH-only reference case, and thus was selected as the basis for use in this update. The newer work translated to 89%, 94%, and 70% conversions of glucan, xylan, and arabinan to their respective monomers, maintaining 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 9% of the original biomass xylan, 1% of the glucan, 25% of the arabinan, 11% of the ash, and 100% of the

acetates, along with solubilizing 26% 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 bioconversion to coproducts. 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, 10]. The power for the subsequent mechanical refining step was set at 200 kWh/dry ton biomass, consistent with vendor inputs provided previously [11].

The present SOT assessment continues the practice of assuming on-site production of enzymes, leveraging the same framework for this operation as originally published in NREL's 2011 ethanol design report and maintained consistently thereafter [2, 10]. As discussed in those reports, we again emphasize that this is *not* to imply that on-site enzyme production would be the optimal practice at commercial scale, but rather is reflected in our models given (a) commercial purchased enzyme costs are impossible to know and state in a public report (being highly business-sensitive information for enzyme companies), and (b) our intent is to transparently capture the true cost of enzyme production in terms of associated capital and operating expenses (alongside the inputs/outputs pertinent to quantifying the carbon intensity for enzyme synthesis). The enzyme cost contribution modeled here is lower than one would expect for an enzyme preparation purchased from a separate, non-adjacent production facility, including concentration, stabilization, and transportation costs (which could be non-trivial), as well as commercial licensing fees (which would be expected regardless of on-site or off-site sourcing, but are not included as any amount would be speculative). Furthermore, by lumping the enzyme production equipment in with the biorefinery, some key items are inherently shared, e.g., the land and buildings, cooling tower, and utilities infrastructure, as well as overhead and fixed costs. Additionally, an external enzyme production facility would probably demand a higher rate of return than the 10% IRR assumed for the biorefinery plant because it is a higher-risk and lower-volume business. Still, in the near term it is more likely that cellulosic biorefineries (whether targeting sugars, ethanol, or hydrocarbons) will purchase enzyme from an external supplier with an organization dedicated to improving enzyme performance and reducing costs – while also providing optimized enzymes with higher activity (as utilized experimentally to generate the SOT data reflected here) than likely expected for a generic *T. reesei* process (as implicit in the TEA model's on-site enzyme production system). Recognizing that external purchase of enzymes at commercial scale would incur higher costs due to both logistical and business economic factors enumerated above, we again reiterate that the TEA results from this assessment do not likely reflect today's "state of the industry" costs, which are expected to be higher with respect to enzyme sourcing (particularly in the near term when there are few commercial cellulosic biorefineries and enzyme companies), relative to n^{th}-plant economics asserted in this SOT analysis.

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 utilized 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 DMR pretreatment given finer and less-filterable particles relative to dilute acid pretreatment. 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/m^2-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 [12].

Bioconversion and Upgrading to Fuels

While further experimental work was conducted over the course of 2022 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 fermentation 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 2019–2022 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 prior recent SOTs 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.

In situ product recovery (ISPR) of acids (membrane pertraction) 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-phosphene-oxide (TOPO) plus 40% undecanone in mineral oil. In the 2019–2022 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). Recently, an engineering subcontract was completed to better understand and refine design and costing details for the ISPR membrane system. The outcomes from that subcontract suggest higher capital and operating costs may realistically be expected for this operation than currently estimated. For consistency across the SOT and design case models, the original ISPR cost estimates are maintained here, but updated costs may be incorporated in future design case iterations (though also noting that alternative strategies are currently being investigated beyond the present ISPR membrane configuration which may reduce costs).

The recovered acids are next subjected to catalytic upgrading, largely maintaining 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 ZrO_2 catalyst at 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 4-heptanone in downstream steps). Relative to prior SOT cases which utilized a weight hourly space velocity (WHSV) of 4.0 h^{-1} in more limited experimental efforts for the ketonization step, more recent experiments over the past year evaluating this operation in greater depth have observed catalyst deactivation by coking and coproduct water inhibition at this WHSV level. Thus, to maintain target catalyst lifetimes, kinetic modeling and further research has shown that in fact this step requires a larger reactor volume consistent with a reduced WHSV of 0.2–0.4 h^{-1}. Accordingly, this metric was adjusted in the present SOT update to 0.4 h^{-1}, increasing both the catalyst and reactor costs relative to prior SOTs (as both of those costs are relatively minimal, ultimately this change increased MFSP by roughly $0.04/GGE relative to what it would otherwise have been in the 2022 SOT).

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 Nb_2O_5 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/Al_2O_3 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, a number of fermentation runs were conducted in 2022, considering both fed-batch operation using clarified/concentrated sugars and batch fermentation on whole slurry hydrolysate (similar to prior historical SOT approaches) using a new organism with improved arabinose utilization capabilities. While the fed-batch approach can achieve significantly higher BDO titers up to 150 g/L versus 70–80 g/L for whole slurry, it requires additional costs for sugar concentration (evaporation) not otherwise employed in the current SOT model configurations. Still, recent TEA modeling has indicated the potential for ultimately reducing net integrated

biorefinery MFSPs through a clarified/concentrated sugar fed-batch fermentation approach given subsequent reductions in water content required to be processed through downstream aqueous BDO upgrading. For current SOT purposes in maintaining a consistent process framework more directly comparable to prior SOT benchmarks, the whole-slurry batch fermentation case was selected for incorporation here. Experimental work for that case made use of a new engineered strain of *Zymomonas mobilis* with improved arabinose utilization capabilities, representing a key advancement in maximizing conversion of available sugar substrates typically present in corn stover hydrolysate. This strain achieved nearly 100% conversion of all three major sugars (glucose, xylose, and arabinose), with nearly 99% metabolic yield to BDO pus acetoin (similar to prior SOTs, acetoin was treated equally to BDO given that either component has been shown to be similarly convertible to desired products through the downstream catalytic upgrading steps). Moreover, substantial conversion of oligomers was also observed during fermentation given the retention of enzymes in the whole-slurry mode of operation, resulting in over 2%, 5%, and 21% increases of glucose, xylose, and arabinose monomers respectively compared to sugar monomers fed to fermentation (experimental data indicated higher conversions than these, but were based on a separate hydrolysis case utilizing higher enzyme loadings of 20 mg/g thus the oligomer conversions were reduced for modeling purposes here). However, these improvements were made at the expense of slower productivity rates, doubling the fermentation batch time from 48 to 96 hours.

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 clean-in-place systems and backwash, before being routed to catalysis steps. For BDO catalytic upgrading, recent experimental data from the 2021 SOT furnished by Oak Ridge National Laboratory (ONRL) collaborators under support of the CUBI consortium were maintained this year. 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 utilized, 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 (2020 SOT) to 100% and 95% (2021 SOT), respectively, based on the recent data from Oak Ridge National Laboratory (ORNL) which indicate 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 over the past year has focused on three major areas for carboxylic acid fermentation: (1) finalizing the build of a pilot-scale reactor, (2) performing pilot-scale (160-L) fermentations to compare to bench-scale fermentations, and (3) generating and evaluating strains of *C. tyrobutyricum* with superior performance. NREL researchers have now finalized construction of the pilot reactor including

rotary ceramic disk filtration unit, progressing cavity pumps, membrane contactors, and a flash distillation unit. Additionally, controls and alarms have been built with this system that will enable automated use and monitoring. This work is in the final stages of commissioning and will begin operations in 2023. This system is anticipated to be able to produce greater than 5 kg of neat butyric acid per run from corn stover hydrolysate.

In preparation for integrated pilot-scale runs with the ISPR system, researchers initiated test fermentations at 160-L scale in conditions used at bench scale. Notably, there was no drop-off in performance during this scale increase, compared to similar conditions at bench scale, suggesting that bench-scale performance can be replicated at the pilot scale. Scale-up performance represented a major risk for this thrust and reducing this risk represents a major accomplishment toward the actualization of this process as a whole.

To date, most of the acid fermentations have involved wildtype strains, however, researchers have developed several lineages of strains that are exhibiting dramatic improvement over wildtype. Leveraging chemical mutagenesis, natural adaptive lab evolution, and rational engineering approaches, several strains have been identified with an enhanced performance in regard to growth rate, pH tolerance, butyric acid productivity and lack of sporulation. Several of these have been proven superior to wildtype strains in bioreactor cultivations and researchers are currently combining promising genetic traits into a single consolidated strain.

Under CUBI efforts for carboxylic acid upgrading, recent research activities focused on evaluating the rate law for short-chain acid ketonization using a downselected commercial ZrO_2 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 CO_2. Coproduct water partial pressure was shown to inhibit the ketonization rate. Additionally, deactivation by coking was found to be more significant than previously understood; a major focus going forward will be to evaluate reactor configurations which will mitigate this issue. 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 $NiMo/Al_2O_3$ pellets that would be 1/20 the price of the baseline Pt/Al_2O_3 catalyst. Complete deoxygenation of the model ketone, 6-undecanone, was observed with crushed $NiMo/Al_2O_3$ pellets under relatively mild conditions (350°C, 1,000-psig H_2), and little to no cracking or isomerization products were observed. 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 [13]. Work planned for next year will focus on transforming neat butyric acid into a wider variety of branched and cyclic jet-range molecules.

For the BDO pathway, preliminary TEA and LCA modeling has identified a promising alternative approach for separating water from the BDO broth prior to catalytic upgrading. To date, one of the primary challenges for the BDO pathway in historical SOTs has been the requirement to process dilute BDO with 90% or higher water content through high-temperature catalytic upgrading, resulting in substantial penalties in capital costs for the aqueous upgrading reactor as well as energy demands for heating up large volumes of BDO/water to catalysis

temperatures (250°C). This has been viewed as a necessity to this point given even higher cost/energy penalties for purifying BDO through conventional distillation approaches, given the need to vaporize large volumes of water from the less-volatile BDO component. However, recent work investigated under both the ChemCatBio (CUBI) and Separations consortia has focused on a pathway involving a reaction of BDO with an aldehyde to yield a dioxolane intermediate, which unlike BDO may be phase-separated from water. The dioxolane intermediate may then (a) undergo steam stripping to revert back to BDO and aldehyde, using a much lower-cost distillation step to recover aldehyde acting in this case as a solvent (reactive extraction) and leaving concentrated BDO to be processed through downstream catalysis; or (b) the dioxolane itself may be sent directly to the same series of catalysis steps as the base case BDO pathway (in this case, the aldehyde becomes a co-reactant alongside BDO). TEA/LCA screening analyses conducted under CUBI and the Separations Consortium have found the potential to maintain or improve both MFSPs and system GHG emissions, potentially by a significant amount, for either processing approach (though requiring that the aldehyde must be obtained from renewable sources in case (b) above in order to maintain a favorable GHG footprint) [14, 15]. This BDO processing approach is still in an earlier stage of development and thus is not incorporated into the present SOT, but will likely be reflected in future design updates as a more optimal configuration.

Lignin Utilization

Relative to prior SOT benchmarks, the 2022 SOT incorporates new data for a modified lignin utilization approach reflecting the latest focus of experimental efforts initially established in the 2021 SOT, 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).

Following a pivot in 2021, experimental work in 2022 continued to focus 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 [16, 17]. 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 [16, 17]. 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 2022 experimental campaign achieved a BKA yield of 1.5 mol BKA/mol lignin aromatics in DMR black liquor, a significant further improvement over 2021 SOT benchmarks at 1.13 mol/mol. In both cases the yields exceeding 100% likely indicate conversion of higher-molecular-weight lignin oligomers or other uncharacterized compounds, thus improving molar yield to the fermentation product by 13-50% relative to prior 2018-2020 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 [18]) was shown to increase nearly threefold, from 0.23 g/L-h in 2021 to 0.65 g/L-h in 2022 – now representing a dramatic tenfold improvement relative to 2020 and prior SOTs with muconic acid at 0.06 g/L-h. 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 maintained 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 [19], 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 may err on the conservative side given the superior properties for downstream product synthesis imparted by BKA versus adipic acid (though countered by a less established market for BKA); thus, higher potential values are also considered as a sensitivity case.

Discussion of Latest R&D Activities and Future Plans

For lignin valorization efforts, realistic paths to this end are being developed in the BETO portfolio to both biofuels and bioproducts, and these paths are likely closely linked together. For example, lignin conversion to fuels will result in jet-fuel-range compounds from distillation, as well as light and heavy compounds from lignin that could be funneled to a single product. Toward this ultimate goal of realistic lignin valorization, 2022 witnessed step changes in multiple fronts.

First, substantial improvements were made for lignin conversion extents to bio-available compounds from realistic lignin substrates in the Lignin Utilization project through the development of industrially relevant oxidation catalysis. This work resulted in the production of >70% of a single valuable product from lignin, which greatly exceeds the literature precedent of roughly 30% of lignin to a single value-added compound. Additionally, significant improvements were also made to lignin monomer recovery and purification, as well as lignin monomer-oligomer fractionation in the Separations Consortium with counter-current chromatography, and in a parallel approach through membrane-based separations. For microbial

conversion of lignin, performance of microbial strains was greatly enhanced for the production of exemplary products like BKA in the Biological Lignin Valorization (BLV) project, incorporated into the SOT updates as discussed above. For lignin fractionation efforts from whole biomass, including woody biomass, the Lignin-First Biorefinery Development project enabled a reduction in organic solvent usage to 1.9 L solvent per kilogram of biomass through novel reaction engineering approaches, which is lower than what is theoretically possible in batch reactors with no solvent recycling. This project is also developing water-only lignin-first biorefining now, and has demonstrated the ability to eliminate the need for exogenous hydrogen gas altogether through solvent-catalyst co-design, all of which can notably reduce the cost and energy consumption of the lignin-first biorefining process. Additionally, the Lignin Conversion to Sustainable Aviation Fuels (SAF) project developed a continuous, solvent-free catalytic process with an Earth-abundant catalyst system (Mo_2C) that allowed for the production of aromatic hydrocarbons from lignin at 86% of theoretical C-mol yield, and TEA and LCA suggested that this approach could be both cost-competitive with today's jet fuels and reduce GHG emissions by up to 70%. The light and heavy cuts from the SAF project are ideally slated for lignin products through oxidation and biological funneling. Overall, in 2023, the work in the Lignin Valorization Platform at NREL will continue with a greater emphasis on process integration at the bench scale, and with a continued focus on further improvements to each unit operation.

Results and Discussion

TEA Results

Based on the details summarized above for experimental performance across the integrated processes, the 2022 SOT benchmark for the **BDO pathway ("burn lignin" scenario)** is estimated at an overall MFSP of **$6.24/GGE total or $4.58/GGE for conversion-related costs (2016 dollars)** excluding feedstock allocations, with feedstock cost maintained at $78.21/dry ton, associated with a 5% ash-equivalent biomass composition as described previously. This corresponds to an overall fuel yield of 47.1 GGE/ton biomass (27.0% 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 $0.38/GGE (6%) lower MFSP relative to last year's 2021 SOT case for the BDO pathway ($6.62/GGE in 2016 dollars) when viewed on comparable footing (i.e., based also on burning lignin in the 2021 case), enabled by improvements in the DMR pretreatment and BDO fermentation steps discussed above..

Similar to the findings in last year's 2021 SOT, the 2022 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 $7.60/GGE for BKA fermentation performance** on hydrolysate. These results are associated with roughly 85% solubilization of residual solid lignin recovered from downstream processing, 24% of which is convertible across lignin fermentation at a BKA process yield of 0.25 g/g total soluble lignin. Given the low fraction of convertible species in the solubilized lignin material, the overall lignin coproduct yields are roughly 24% of their final 2030 targets (on a mass basis), which combined with 35% 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 break-even point with combustion, **improvements to BKA production enabled a net MFSP reduction of $1.05/GGE (12%)** for the 2022 SOT BDO pathway relative to prior 2021 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 **$7.02/GGE total or $5.06/GGE for conversion-related costs (2016 dollars)** excluding feedstock allocations is estimated for the 2022 SOT. This corresponds to an overall fuel yield of 40.0 GGE/ton biomass (23.4% 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 2021 SOT baseline at $7.07/GGE, strictly as a function of improvements to pretreatment and enzymatic hydrolysis yields (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 $8.61/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 2021 SOT results for the "base case" lignin coproduct scenario producing adipic acid, this leads **to reductions of $0.72/GGE (8%)**, again enabled by improvements to the bioconversion rate and yield of BKA coproduct from lignin compared to the 2021 SOT.

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 $7.48/GGE for the BDO pathway or $8.47/GGE for the acids pathway**, while at a **20% premium** ($1.03/lb), the **MFSP would reduce further to $7.37/GGE or $8.33/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 fourfold higher than current SOT benchmarks.

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2022 SOT	2022 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]	Burn Lignin	Convert Lignin: BKA [a]	Convert Lignin
Projected MFSP	$/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	$6.24	$7.60	$2.47
Feedstock contribution	$/GGE	$2.67	$2.59	$2.59	$2.11	$2.11	$1.93	$1.93	$1.83	$1.83	$1.66	$1.66	$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	$4.58	$5.93	$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	47.1	47.1	43.2
Adipic acid [BKA] coproduct yield	lb/dry ton biomass	0	0	40	0	42	0	39	0	[47]	0	[63]	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	$78.21	$78.21	$71.26
Pretreatment													
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids loading	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	90	90	90	90	90	90	90	90	92
Reactor mode	Batch vs. counter-current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter-current
Total loading: NaOH [Na$_2$CO$_3$]	mg/g dry biomass	70	70	70	80	80	24 [80]	24 [80]	24 [80]	24 [80]	33 [90]	33 [90]	70
Net solubilized lignin to liquor	%	47%	47%	47%	50%	50%	20%	20%	20%	20%	26%	26%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	3%	3%	3%	3%	1%	1%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	16%	16%	12%	12%	12%	12%	9%	9%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	48%	48%	48%	48%	25%	25%	30%
Enzymatic Hydrolysis													
Hydrolysis configuration	Batch vs. CEH	Batch	Batch	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%	20%	20%	25%
Enzymatic hydrolysis batch time	days	5	5	5	5	5	7	7	7	7	6	6	5
Hydrolysis glucan to glucose	%	78%	78%	78%	84%	84%	88%	88%	88%	88%	89%	89%	90%
Hydrolysis xylan to xylose	%	85%	85%	85%	82%	82%	93%	93%	93%	93%	94%	94%	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)	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	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	0.83	0.83	2.6

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2022 SOT	2022 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]	Burn Lignin	Convert Lignin: BKA [a]	Convert Lignin
Glucose to product [total glucose utilization] [c]	%	86% [100%]	95% [100%]	95% [100%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	96% [99.6%]	99% [100%]	99% [100%]	95% [98%]
Xylose to product [total xylose utilization] [c]	%	89% [97%]	90% [92%]	90% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	89% [92%]	96% [97%]	96% [97%]	90% [92%]
Arabinose to product [total arabinose utilization] [c]	%	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	0% [0%]	99% [100%]	99% [100%]	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]	0.48 [0.47]	0.48 [0.47]	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%	97.2%	97.2%	96.4%
Aqueous BDO upgrading: WHSV	h^{-1}	1	1	1	1	1	1	1	2	2	2	2	2
Aqueous BDO upgrading: per-pass conversion	wt % to desired products	89%	90%	90%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Oligomerization: WHSV	h^{-1}	1	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%	100%	100%
Hydrotreating: WHSV	h^{-1}	5	5	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%	100%	100%
Lignin Processing to Coproduct													
Solid deconstruction to soluble lignin	wt % BCD lignin feed	-	-	85% [e]	-	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%	-	24%	98%
Fermentation process yield from lignin	g/g soluble lignin	-	-	0.15	-	0.16	-	0.16	-	0.19	-	0.25	1.59
Fermentation metabolic yield from lignin	g/g lignin monomers	-	-	0.93	-	0.93	-	0.93	-	1.19	-	1.58	0.93
Overall carbon upgrading efficiency to coproduct [d]	mol %	-	-	3.8%	-	3.8%	-	4.0%	-	5.4%	-	7.2%	27.8%
Fermentation productivity	g/L/h	-	-	0.06 (0.53)	-	0.06 (0.53)	-	0.06 (0.53)	-	0.23	-	0.65	1
Coproduct production	MMlb/yr	-	-	29	-	30	-	29	-	34	-	46	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. 2021-2022 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 INL 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.

Table 2(b). Acids Pathway: Technical Summary Table for 2022 SOT Benchmark, 2017–2021 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	2022 SOT	2022 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]	Burn Lignin	Convert Lignin: BKA [a]	Convert Lignin
Projected MFSP	$/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	$7.02	$8.61	$2.49
Feedstock contribution	$/GGE	$3.19	$2.99	$2.99	$2.30	$2.30	$2.08	$2.09	$2.03	$2.04	$1.95	$1.96	$1.59
Conversion contribution	$/GGE	$7.86	$7.41	$11.67 ($10.17)	$5.90	$9.17 ($7.98)	$5.04	$7.93 ($6.96)	$5.04	$7.29	$5.06	$6.65	$0.90
Total gasoline equivalent yield	GGE/dry U.S. ton	26.3	28	28	35.3	35.3	38.5	38.4	38.5	38.4	40.0	40.0	44.8
Adipic acid [BKA] coproduct yield	lb/dry ton biomass	0	0	41	0	42	0	40	0	[48]	0	[64]	259
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	$78.21	$78.21	$71.26
Pretreatment													
Method	-	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR	DMR
Solids loading	wt %	20%	20%	20%	20%	20%	20%	20%	20%	20%	20%	20%	30%
Temperature	°C	92	92	92	90	90	90	90	90	90	90	90	92
Reactor mode	Batch vs. counter-current	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Batch	Counter-current
Total loading: NaOH [Na$_2$CO$_3$]	mg/g dry biomass	70	70	70	80	80	24 [80]	24 [80]	24 [80]	24 [80]	33 [90]	33 [90]	70
Net solubilized lignin to liquor	%	47%	47%	47%	50%	50%	20%	20%	20%	20%	26%	26%	47%
Net solubilized glucan to liquor	%	2%	2%	2%	2%	2%	3%	3%	3%	3%	1%	1%	2%
Net solubilized xylan to liquor	%	17%	17%	17%	16%	16%	12%	12%	12%	12%	9%	9%	10%
Net solubilized arabinan to liquor	%	46%	46%	46%	46%	46%	48%	48%	48%	48%	25%	25%	30%
Enzymatic Hydrolysis													
Hydrolysis configuration	Batch vs. CEH	Batch	Batch	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%	20%	20%	7.60%
Enzymatic hydrolysis batch time	days	5	5	5	5	5	7	7	7	7	6	6	Continuous
Hydrolysis glucan to glucose	%	78%	78%	78%	84%	84%	88%	88%	88%	88%	89%	89%	96%
Hydrolysis xylan to xylose	%	85%	85%	85%	82%	82%	93%	93%	93%	93%	94%	94%	99%
Sugar loss (into solid stream after EH separation)	%	5%	5%	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	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	0.62	0.62	2
Glucose to product [total glucose utilization] [c]	%	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% [97.5%]	95% [97.5%]	95% [100%]
Xylose to product [total xylose utilization] [c]	%	82% [100%]	77% [90%]	77% [90%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	95% [97.5%]	85% [100%]

	Units	2017 SOT	2018 SOT	2018 SOT	2019 SOT	2019 SOT	2020 SOT	2020 SOT	2021 SOT	2021 SOT	2022 SOT	2022 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]	**Burn Lignin**	**Convert Lignin: BKA** [a]	**Convert Lignin**
Arabinose to product [total arabinose utilization] [c]	%	82% [100%]	32% [38%]	32% [38%]	20% [29.0%]	20% [29.0%]	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 [0.44]	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	76% C2, 98% C4	76% C2, 98% C4	100% (C4)
Ketonization: WHSV	h^{-1}	6	4	4	4	4	4	4	4	4	0.4	0.4	6
Ketonization: per-pass conversion	wt % to desired products	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%	100%
Condensation: WHSV	h^{-1}	0.5	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	10-h res. time	15-h batch
Condensation: overall conversion	wt % to desired products	81%	92%	92%	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	4.7	4.7	3
Hydrotreating: per-pass conversion	wt % to desired products	100%	100%	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]	-	85%[5]	53%
Convertible components in soluble lignin	wt % of total soluble lignin (APL + BCD)	-	-	16%	-	16%	-	16%	-	18%	-	24%	98%
Fermentation process yield from lignin	g/g soluble lignin	-	-	0.15	-	0.16	-	0.16	-	0.19	-	0.25	1.59
Fermentation metabolic yield from lignin	g/g lignin monomers	-	-	0.93	-	0.93	-	0.93	-	1.19	-	1.58	0.93
Overall carbon upgrading efficiency to coproduct [d]	mol %	-	-	4.0%	-	4.0%	-	4.0%	-	5.4%	-	7.2%	30.1%
Fermentation productivity	g/L/h	-	-	0.06 (0.53)	-	0.06 (0.53)	-	0.06 (0.53)	-	0.23	-	0.65	1
Coproduct production	MMlb/yr	-	-	30	-	31	-	29	-	35	-	46	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. 2021-2022 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 INL 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.

Table 2 and Figure 2 also show the detailed comparisons between the 2022 SOT scenarios, the 2017–2021 prior SOTs, and the future design case targets moving forward to achieving <$2.50/GGE by 2030. Moving forward to those future out-year projections, many parameters have now met or exceeded their targets, though more 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 89% 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, or any other pathway involving clarified sugar fermentations, the CEH concept offers substantial potential to further improve overall biorefinery economics by improving sugar yields and/or reducing enzyme loadings, as well as offering the ability to recycle enzymes for multiple uses, while also directly incorporating solid/liquid separation without the need for added flocculants (and currently unknown impact they may impart on downstream lignin processing operations).

Sugar fermentation and catalytic upgrading performance may also be improved beyond 2022 SOT benchmarks. In the BDO pathway, fermentation yields have now surpassed final 2030 goals (on whole-slurry hydrolysate), including capabilities for arabinose utilization, though fermentation productivity may still be improved. 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 (such as the dioxolane pathway discussed above). 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).

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 calling for further improvements in ketonization WHSV (particularly in light of the latest findings for WHSV now being much lower than previously understood) 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 bioconversion productivity (translating to larger fermentor volumes and costs for this aerobic fermentation step, though this has improved substantially over the past two years), 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 59% since SOT tracking began for lignin conversion, while also improving fermentation productivity roughly tenfold over prior muconic/adipic acid benchmarks. Still, relative to 2021 SOT levels, the lignin train must improve by 2030 to achieve a further 50% improvement in productivity (from 0.65 up to 1.0 g/L-h) and sixfold improvement in overall lignin conversion (from 0.25 to 1.6 g/g soluble lignin process yields) in order to improve overall coproduct outputs from 46 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 as currently configured 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 as well as GHG improvements through other processing approaches (based on experimental efforts being undertaken in such areas). Leading options for such strategies are discussed further below.

Figure 2 provides a waterfall plot of MFSP cost breakdowns by process area, reflecting the key cases listed in Table 2.
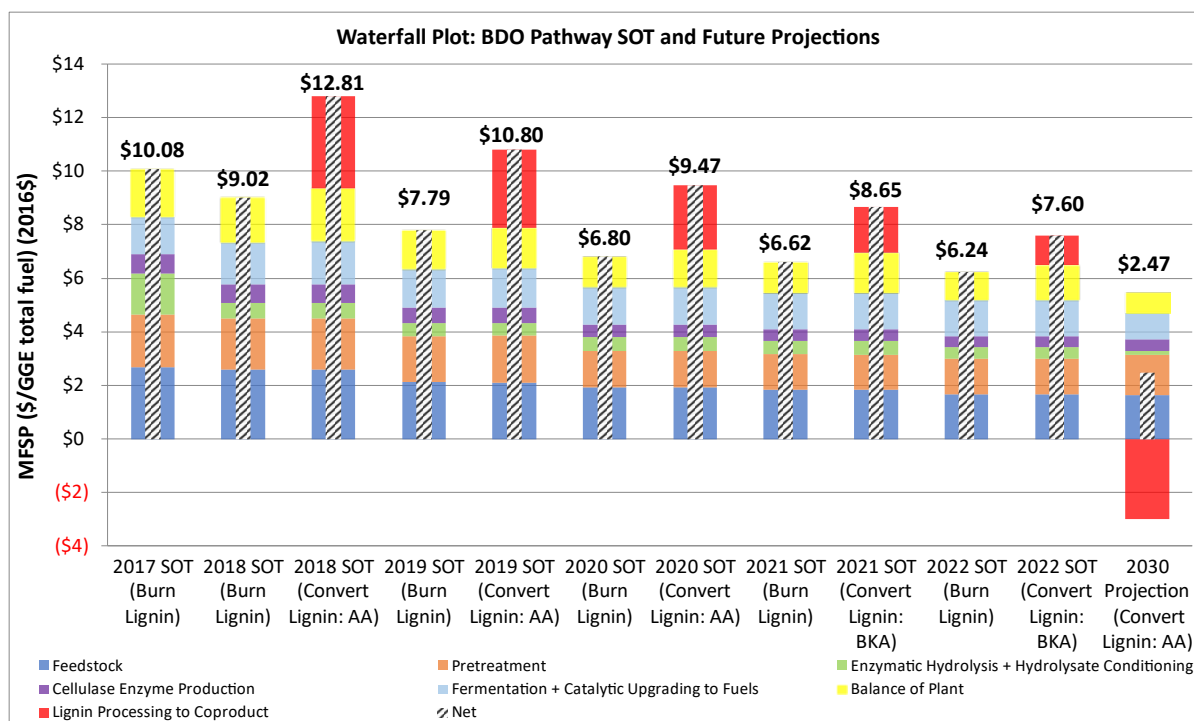
Figure 2(a). Tracking SOT progression from 2017–2022, compared to out-year 2030 projection (BDO pathway)
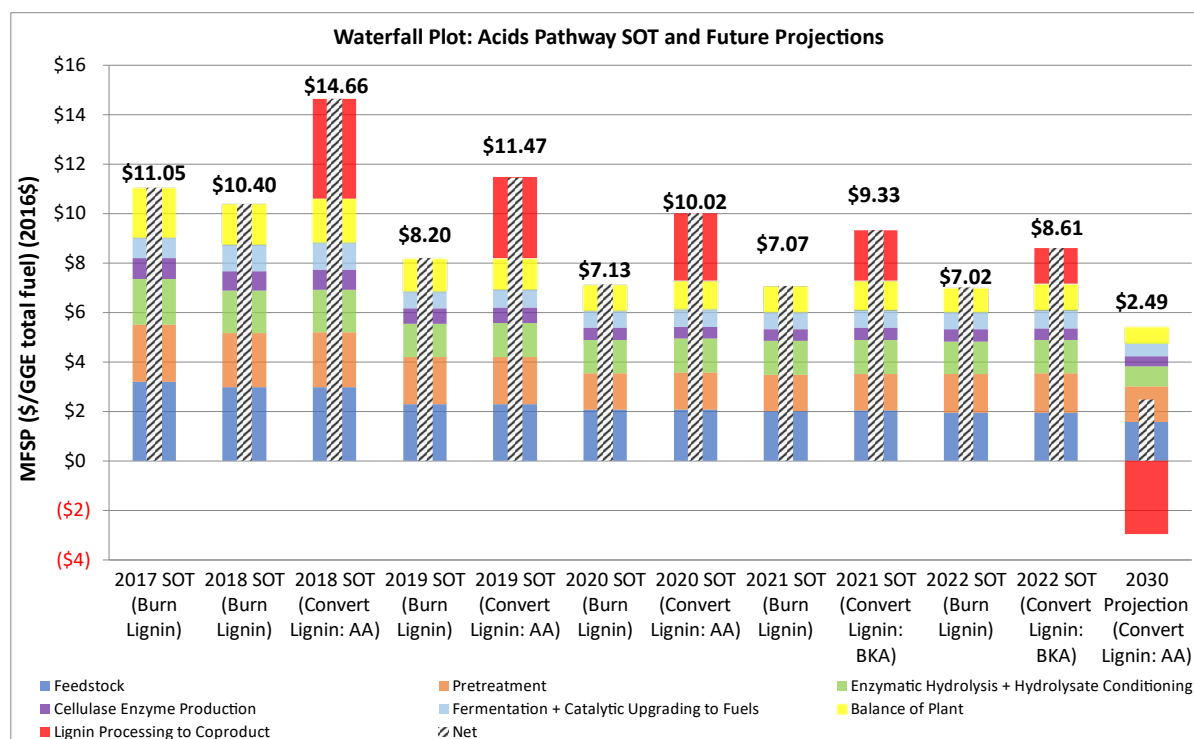
Figure 2(b). Tracking SOT progression from 2017–2022, compared to out-year 2030 projection (acids pathway)

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 notable increase in mass/carbon yield to fuels for the 2022 SOT case relative to 2021 attributed to improved BDO fermentation yields and to slightly higher sugar yields from the latest DMR updates, while the acids pathway reflects more minimal improvements in these metrics compared to 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 in 2021 to lignin conversion to BKA rather than muconic/adipic acid, natural gas demands were increased over prior levels due to higher energy requirements for BKA product recovery/purification. Water consumption per GGE fuel decreased for both lignin scenarios in 2022 compared to 2021 benchmarks following trends in fuel yield improvements.

Table 3. Sustainability Indicators for 2017–2022 SOT and Future Projection Scenario

	2017 SOT Burn Lignin	2018 SOT Burn Lignin	2018 SOT Convert Lignin	2019 SOT Burn Lignin	2019 SOT Convert Lignin	2020 SOT Burn Lignin	2020 SOT Convert Lignin	2021 SOT Burn Lignin	2021 SOT Convert Lignin: BKA	2022 SOT Burn Lignin	2022 SOT Convert Lignin: BKA	2030 Projection Convert Lignin
BDO 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%	14.3%	14.3%	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%	27.0%	27.0%	25.0%
Carbon efficiency to lignin coproduct (% feedstock C)	NA	NA	2.3%	NA	2.3%	NA	2.2%	NA	2.4%	NA	3.2%	14.8%
Net electricity import (kWh/GGE)	12.3	5.1	14.0	5.7	12.5	4.9	11.4	6.3	10.6	7	10.5	10.5
Net natural gas import (Btu/GGE [LHV][a])	0	0	75,284	0	69,928	0	60,607	0	85,593	0	82,834	14,596
Water consumption (gal water/GGE)	23.4	13.9	11.3	10.9	9.2	9.3	7.8	8.0	10.1	6.8	8.9	8.9
Acids Pathway												
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%	12.3%	12.3%	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%	23.4%	23.3%	26.2%
Carbon efficiency to lignin coproduct (% feedstock C)	NA	NA	2.3%	NA	2.3%	NA	2.2%	NA	2.4%	NA	3.2%	14.4%
Net electricity import (kWh/GGE)	5.8	1.3	21.5	2.8	17.4	2.2	15.5	2.2	16.4	2.6	16.1	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	10,727	16,438	9,055
Water consumption (gal water/GGE)	30.7	36.0	26.0	27.7	20.0	24.7	17.9	24.7	19.7	23.4	18.3	13.5

[a] Lower heating value

Discussion: Considerations for Future Priorities

Over the past three years, substantial progress has been made spanning all key areas of the integrated biochemical design case pathways as highlighted herein. The associated technical progress has translated to notable progress in both TEA metrics (documented here) as well as LCA metrics (quantified in ANL's accompanying *Supply Chain Sustainability Analysis* reports [20]), with the latter increasing in priority moving forward to benchmark and improve upon carbon intensity metrics for pathways of focus. Relative to the 2018 NREL design report projections for 2030 targets [21], progress is largely on track and in many cases meeting or exceeding final goals. While lignin deconstruction and upgrading remains the largest area of further required improvement relative to the original 2030 goals, substantial progress has also been made there particularly over the past two years. Accordingly, we have achieved our 3-year project milestone by exceeding the 2022 MFSP projections previously set in our 2021 Go/No-Go milestone, targeting $8.98/GGE and $9.04/GGE for the BDO and acids pathways respectively (based on the lignin conversion scenarios), and in fact have also surpassed the 2023 goals one year early relative to those prior out-year projections [22].

However, recent shifts in programmatic priorities for BETO create opportunities for revisiting or further optimizing design case pathways moving forward, particularly with respect to:
   a) Increased prioritization for deep decarbonization to maximize GHG reductions relative to petroleum fuel benchmarks
   b) Maximizing production of SAF for biofuel-focused pathways
   c) Further considerations for process complexity, scale-up risk, and other barriers to near-term deployment, supplemented by additional guidance through industry engagement

In light of the above priorities and insights gained through TEA/LCA screening of additional biorefinery pathway approaches conducted under this project over recent years, several opportunities exist for further analysis moving into 2023 and beyond, ultimately in support of establishing updated design cases planned to be a key focus in the coming year. Though not intended to be an exclusive list, leading options for consideration moving forward include:

   1) **Alternative approaches to optimize pretreatment and lignin fractionation:** Recent TEA/LCA analysis has identified encouraging potential to achieve better lignin fractionation with favorable cost and GHG metrics through reductive catalytic fractionation (RCF) processes [23]. In particular, RCF configured to process residual lignin-rich streams downstream of pretreatment, making use of butanol/water solvent mixtures and improving separations strategies, exhibits potential for optimal TEA/LCA outcomes in the context of an integrated biorefinery seeking to maximize the utilization of lignin for either fuels (SAF) or value-added products. For example, recent analyses have shown the potential for SAF to be produced from residual lignins via RCF and subsequent hydrodeoxygenation with up to 81% GHG emissions reduction versus petroleum derived jet fuel at a SAF selling price of $2.52/GGE while producing sugars from carbohydrates at $0.33/lb [24].

   2) **Modified BDO pathway:** Experimental and TEA/LCA assessment activities for the BDO pathway have recently shifted to focus on purifying BDO without the need for energy-intensive distillation via reaction to a dioxolane intermediate (discussed above). Initial findings under both the ChemCatBio and Separations consortia have highlighted encouraging potential to substantially reduce GHG emissions while maintaining or also improving economics through the dioxolane route, with one study identifying over 15% GHG reduction potential at comparable economics [15] and another study estimating 45% GHG reduction and 35% MFSP reduction potential relative to current benchmarks [14]. This would represent a significant improvement over the current approach, with further room to investigate modifications around BDO catalysis to shift the fuel outputs from diesel to SAF.

   3) **Modified acids pathway:** Likewise, more recent work conducted under the ChemCatBio consortium has focused on wet waste upgrading via arrested anaerobic digestion to mixed volatile fatty acids. This approach offers several advantages over the current biochemical SOT pathway, primarily (a) eliminating the need for a condensation step (reducing the number of catalysis steps from three to two), and (b) maximizing hydrocarbon components in the boiling range ideally suited for SAF. While the wet waste process does not fit directly into the biochemical SOT framework focused on terrestrial biomass feedstocks, learnings gained from the work on that pathway may be applied here—e.g., in

targeting a similar mixture of carboxylic acids from sugar fermentation organisms to enable similar catalysis chemistries. Additionally, further opportunities exist to improve the acid recovery operation. We have recently completed an engineering subcontract to refine the fidelity of the design/cost details for *in situ* product removal of the acids via pertraction, which may either be incorporated into future iterations of this pathway or otherwise replaced with a lower-cost approach for acids recovery.

4) **Catalytic upgrading of sugars to fuels:** In 2021, NREL published a technical report documenting a new strategy for direct catalytic upgrading of biomass sugars to hydrocarbon fuels via dehydration to furans followed by aldol condensation and hydrotreating [25]. TEA modeling for the pathway demonstrated the potential to achieve MFSPs on-par with the BDO and acids pathways when assuming the same targets for lignin valorization to coproducts ($2.5–$2.7/GGE depending on sourcing for a ketone co-reactant), while achieving significantly higher fuel yield potential over 60 GGE/ton of biomass. One key challenge for this pathway was a significant demand for natural gas due to high loading of an expensive solvent (dioxane) required in the dehydration step, incurring large temperature swings and thus high heating and cooling requirements. More recently, work under the ChemCatBio consortium has identified more optimal conditions switching to a lower-cost acetone solvent more easily recovered while avoiding the prior temperature swings, leading to a reduction of roughly 50% or greater in natural gas consumption (a leading driver in overall system GHG emissions) and an MFSP potential better than either of the biological design case pathways. Similarly, a prior design case published in 2015 evaluated a separate catalytic upgrading pathway based on aqueous phase reforming of sugars to hydrocarbon fuels [11], also highlighting the potential to achieve higher fuel yields and lower MFSPs than all biological pathways we have evaluated to date.

5) **Ethanol-to-jet:** From strictly a TEA and LCA perspective, the most promising biological pathway to SAF that we have investigated remains ethanol-to-jet (ETJ). The ETJ pathway achieves higher metabolic energy yields, and ultimately higher energy-equivalent fuel yields after catalytic upgrading, than many other biological/catalytic pathways from sugars to fuels including the BDO and acids design case pathways, while greatly reducing process complexity and avoiding key challenges with the design case pathways tied to intermediate recovery steps. Moreover, ETJ may be more readily deployable in the near term based on higher-technology-readiness-level (TRL) technologies while supporting a means to tie in to the established ethanol industry for expanding to new fuel opportunities. Recent TEA/LCA modeling under this project has highlighted the potential to reduce MFSP by nearly $0.50/GGE for an ETJ approach compared to the BDO and acids design case pathways when evaluated under the same integrated biorefinery framework, while also reducing GHG emissions by roughly 15% [26].

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 2022 experimental work on integrated hydrolysate processing, the 2022 SOT considers two bioconversion pathways for hydrocarbon fuel production, namely BDO and carboxylic acids. Biomass deconstruction efforts have further improved upon prior performance at 89% glucan conversion, 94% xylan conversion, and 70% arabinan conversion to monomeric sugars through saccharification at 10-mg/g total enzyme loading, enabled by a more optimal two-stage DMR pretreatment approach making use of sodium carbonate to reduce more costly sodium hydroxide usage (also yielding notable LCA improvements). Sugar fermentation performance was also improved over prior SOT levels for the BDO pathway, utilizing nearly 100% of glucose, xylose, and (new in 2022) arabinose sugars at nearly 100% metabolic yields to BDO and acetoin, though at the expense of lower productivities. Performance for aqueous BDO catalytic upgrading was not further improved beyond 2021 levels, thus 2021 SOT benchmarks were maintained for those operations, although promising new directions were identified through BDO conversion to a dioxolane intermediate paving the way for future cost and energy reductions for BDO conversion to fuels. Similarly, performance benchmarks were maintained from recent SOTs for the acids pathway through fermentation and catalytic upgrading, with the exception of reduced WHSV for acid ketonization reflecting recent learnings on catalyst inhibition from coproduced water. **The resulting 2022 SOT benchmark MFSPs are estimated to be $6.24/GGE and $7.02/GGE ($4.58/GGE and $5.06/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 2021 SOT basis, this translates to an improvement of $0.38/GGE and $0.05/GGE in overall MFSPs for the two respective pathways.

Building from improvements in lignin conversion to coproducts demonstrated in 2021 with a shift to more optimal BKA production in place of muconic/adipic acid, lignin monomer fermentation performance was considerably improved in 2022 leading to further notable MFSP reductions on the order of $0.72–$1.05/GGE. **The 2022 SOT MFSPs are estimated at $7.60/GGE and $8.61/GGE for lignin conversion** on biomass-derived substrates (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). However, this gap has continued to shrink toward a break-even point with lignin combustion, owing to a 33% improvement in fermentation yield and nearly threefold improvement in productivity demonstrated in 2022 relative to 2021 BKA benchmarks. If BKA market prices could fetch a premium over adipic acid given BKA's property/performance advantages, these MFSPs could be reduced by roughly $0.12–$0.28/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 14.3% by weight or 27.0% by carbon retention relative to biomass feedstock, along with 3.2% carbon yields to BKA coproduct in the "convert lignin" scenarios. Fuel yields are slightly lower for the acids case at 12.3% by weight or 23.3% by carbon utilization, with the same 3.2% carbon yield basis to BKA. Net power imports are calculated as 7.0 kWh/GGE for the BDO case or 2.6 kWh/GGE for the acids case in the "burn

lignin" scenario, increasing to 10.5 and 16.1 kWh/GGE, respectively, in the "convert lignin" scenario (driven in large part by power demands for aerobic lignin). Approximately 83,000 Btu/GGE of supplemental natural gas is required for the 2022 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 16,000 BTU/GGE for the "convert lignin" scenario. Finally, water consumption is estimated at 6.8 gal/GGE for the BDO "burn lignin" case, and roughly 8.9 gal/GGE for the BDO "convert lignin" case. Water consumption is higher at 23.4 gal/GGE in the acids "burn lignin" case, reducing to 18.3 gal/GGE in the "convert lignin" case, driven in part by still requiring the hydrolysate solid/liquid separation and water wash step.

Overall, both SOT pathways have demonstrated considerable progress over the past three years, exceeding previously set 2022 goals and in many cases meeting or surpassing 2030 projections. Namely, biomass deconstruction to sugars has demonstrated high yields at low enzyme loadings through DMR pretreatment and enzymatic hydrolysis, while also substantially reducing energy-intensive sodium hydroxide demands through a more optimal two-stage alkali extraction approach. Fermentation and catalytic upgrading for both fuel pathways have also largely met 2030 goals, with the exception of productivity rates (though for anaerobic fermentation the remaining productivity gains do not represent significant cost impacts) and arabinose utilization in the case of the acids pathway. Finally, considerable progress has also been made around lignin upgrading to coproducts, primarily through bioconversion yields and productivity rates, though continued improvements would be required in the lignin processing 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. Given future directions shifting to prioritizing deeper GHG reductions, maximizing SAF, and targeting near-term deployment potential, a number of opportunities exist to re-configure the current SOT pathways or otherwise to move to new pathways, for which a new design report update will be established moving forward.

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Appendix A. TEA Summary Sheets for 2022 SOT Benchmark Models (2016 dollars)

BDO Pathway (Burn Lignin)

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

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

Minimum Fuel Selling Price (MFSP, Gasoline-Equivalent Basis):		**$6.24 /GGE**
Contributions:	Feedstock	**$1.66 /GGE**
	Fuel Conversion	**$4.58 /GGE**
	Coproduct Conversion	**$0.00 /GGE**

Fuel Production	34.1 MMGGE per year (at 68 °F)
Fuel Yield	47.0 GGE / dry U.S. ton feedstock
BKA Coproduct Yield	0 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield]	0.47 [0.5] kg BDO/kg Total Sugars (95% of theoretical)
Feedstock + Handling Cost	$78.21 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs

Area 200: Pretreatment	$51,494,495
Area 300: Sugar Hydrolysis and Conditioning	$23,560,948
Area 400: Enzyme Production	$11,531,386
Area 500: Bioconversion and Upgrading	$79,451,043
Area 600: Wastewater	$55,545,375
Area 700: Lignin	$0
Area 800: Boiler	$62,389,921
Area 900: Utilities & Storage	$12,181,134
Total Installed Equipment Cost	**$296,154,302**
Added Direct + Indirect Costs	$252,045,698
(% of TCI)	46%
Total Capital Investment (TCI)	**$548,200,000**
Installed Equipment Cost/Annual GGE	$8.69
Total Capital Investment/Annual GGE	$16.09
Operating Hours Per Year (On-Stream Factor)	7884 (90%)
Loan Rate	8.0%
Term (years)	10
Capital Charge Factor (Computed)	0.129
Fuel Carbon Retention Efficiencies:	
From Hydrolysate Sugar (Fuel C / Sugar C)	52.6%
From Biomass (Fuel C / Biomass C)	27.0%
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]	103,802
Current Yield (Actual/Theoretical)	68.7%

[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	166.3
Sulfuric Acid	0.0
Caustic	33.4
Sodium Carbonate	32.6
Glucose (enzyme production)	25.0
Hydrogen	35.2
Electricity (import)	46.6
Other Raw Materials	67.5
Catalysts	8.7
Waste Disposal	4.2
Na2SO4 Coproduct	-45.6
BKA coproduct ($0.86/lb)	0.0
Fixed Costs	43.2
Capital Depreciation	50.8
Average Income Tax	15.7
Average Return on Investment	140.4
Total	**624.2**

Manufacturing Costs ($/yr)

Feedstock + Handling	$56,700,000
Sulfuric Acid	$0
Caustic	$11,400,000
Glucose (enzyme production)	$8,500,000
Hydrogen	$12,000,000
Electricity (import)	$15,900,000
Other Raw Materials	$23,000,000
Catalysts	$3,000,000
Waste Disposal	$1,400,000
Na2SO4 Coproduct	-$15,500,000
BKA coproduct ($0.86/lb)	$0
Fixed Costs	$14,700,000
Capital Depreciation	$17,300,000
Average Income Tax	$5,400,000
Average Return on Investment	$47,900,000
Total	**$201,700,000**

Specific Operating Conditions

Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	7.0
Plant Electricity Use (kWh/GGE)	11.8

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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):	**$7.60 /GGE**

Contributions:	Feedstock	**$1.66 /GGE**
	Fuel Conversion	**$4.82 /GGE**
	Coproduct Conversion	**$1.12 /GGE**

Fuel Production	34.1 MMGGE per year (at 68 °F)
Fuel Yield	47.1 GGE / dry U.S. ton feedstock
BKA Coproduct Yield	63 lb / dry U.S. ton feedstock
2,3-Butanediol Process Yield [Theoretical Yield]	0.47 [0.5] kg BDO/kg Total Sugars (95% of theoretical)
Feedstock + Handling Cost	$78.21 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	$51,438,663
Area 300: Sugar Hydrolysis and Conditioning	$23,560,922
Area 400: Enzyme Production	$11,531,386
Area 500: Bioconversion and Upgrading	$79,538,243
Area 600: Wastewater	$56,106,939
Area 700: Lignin	$200,288,523
Area 800: Boiler	$54,266,243
Area 900: Utilities & Storage	$13,749,108
Total Installed Equipment Cost	$490,480,027
Added Direct + Indirect Costs	$443,119,973
(% of TCI)	47%
Total Capital Investment (TCI)	$933,600,000
Installed Equipment Cost/Annual GGE	$14.39
Total Capital Investment/Annual GGE	$27.39
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)	52.6%
From Biomass (Fuel C / Biomass C)	27.0%
BKA Carbon Efficiency from Biomass	3.2%
Maximum Yields (100% of Theoretical)[a]	
Fuel Production (U.S. ton/yr)	151,073
Current Fuel Production (U.S. ton/yr)[b]	103,849
Current Yield (Actual/Theoretical)	68.7%

[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	166.2
Sulfuric Acid	27.4
Caustic	55.3
Sodium Carbonate	32.6
Glucose (enzyme production)	25.0
Hydrogen	35.3
Electricity (import)	70.0
Other Raw Materials	90.7
Catalysts	9.3
Waste Disposal	4.3
Na2SO4 Coproduct	-59.6
BKA coproduct ($0.86/lb)	-115.4
Fixed Costs	68.4
Capital Depreciation	86.9
Average Income Tax	26.3
Average Return on Investment	237.1
Total	759.7

Manufacturing Costs ($/yr)	
Feedstock + Handling	$56,700,000
Sulfuric Acid	$9,300,000
Caustic	$18,900,000
Glucose (enzyme production)	$8,500,000
Hydrogen	$12,000,000
Electricity (import)	$23,800,000
Other Raw Materials	$30,900,000
Catalysts	$3,200,000
Waste Disposal	$1,400,000
Na2SO4 Coproduct	-$20,300,000
BKA coproduct ($0.86/lb)	-$39,300,000
Fixed Costs	$23,300,000
Capital Depreciation	$29,600,000
Average Income Tax	$9,000,000
Average Return on Investment	$80,800,000
Total	$247,800,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	10.5
Plant Electricity Use (kWh/GGE)	12.9

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):	**$7.02 /GGE**

Contributions:	Feedstock	**$1.95 /GGE**
	Fuel Conversion	**$5.06 /GGE**
	Coproduct Conversion	**$0.00 /GGE**

Fuel Production	29.0 MMGGE per year (at 68 °F)
Fuel Yield	40.0 GGE / dry U.S. ton feedstock
BKA Coproduct Yield	0 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.44 [0.49] kg Acid/kg Total Sugars (89% of theoretical)
Feedstock + Handling Cost	$78.21 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	$51,494,495
Area 300: Sugar Hydrolysis and Conditioning	$83,977,215
Area 400: Enzyme Production	$11,531,386
Area 500: Bioconversion and Upgrading	$53,673,311
Area 600: Wastewater	$60,423,837
Area 700: Lignin	$0
Area 800: Boiler	$69,021,175
Area 900: Utilities & Storage	$12,008,465
Total Installed Equipment Cost	$342,129,885
Added Direct + Indirect Costs	$293,470,115
(% of TCI)	46%
Total Capital Investment (TCI)	$635,600,000
Installed Equipment Cost/Annual GGE	$11.80
Total Capital Investment/Annual GGE	$21.93
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)	47.9%
From Biomass (Fuel C / Biomass C)	23.4%
BKA Carbon Efficiency from Biomass	0.0%
Maximum Yields (100% of Theoretical)[a]	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr)[b]	88,926
Current Yield (Actual/Theoretical)	69.0%

[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	195.4
Sulfuric Acid	0.0
Caustic	39.3
Sodium Carbonate	38.4
Glucose (enzyme production)	29.4
Hydrogen	0.0
Electricity (import)	16.1
Other Raw Materials	92.0
Catalysts	2.8
Waste Disposal	4.9
Na2SO4 Coproduct	-52.7
BKA coproduct ($0.86/lb)	0.0
Fixed Costs	56.4
Capital Depreciation	69.3
Average Income Tax	21.2
Average Return on Investment	189.0
Total	701.6

Manufacturing Costs ($/yr)	
Feedstock + Handling	$56,700,000
Sulfuric Acid	$0
Caustic	$11,400,000
Glucose (enzyme production)	$8,500,000
Hydrogen	$0
Electricity (import)	$4,700,000
Other Raw Materials	$26,700,000
Catalysts	$800,000
Waste Disposal	$1,400,000
Na2SO4 Coproduct	-$15,300,000
BKA coproduct ($0.86/lb)	$0
Fixed Costs	$16,400,000
Capital Depreciation	$20,100,000
Average Income Tax	$6,100,000
Average Return on Investment	$54,800,000
Total	$192,300,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	2.6
Plant Electricity Use (kWh/GGE)	15.2

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):	**$8.61 /GGE**

Contributions:	Feedstock	**$1.96 /GGE**
	Fuel Conversion	**$5.21 /GGE**
	Coproduct Conversion	**$1.44 /GGE**

Fuel Production	28.9 MMGGE per year (at 68 °F)
Fuel Yield	40.0 GGE / dry U.S. ton feedstock
BKA Coproduct Yield	64 lb / dry U.S. ton feedstock
Butyric Acid Process Yield [Theoretical Yield]	0.44 [0.49] kg Acid/kg Total Sugars (89% of theoretical)
Feedstock + Handling Cost	$78.21 /dry U.S. ton feedstock
Internal Rate of Return (After-Tax)	10%
Equity Percent of Total Investment	40%

Capital Costs	
Area 200: Pretreatment	$51,494,495
Area 300: Sugar Hydrolysis and Conditioning	$83,977,215
Area 400: Enzyme Production	$11,531,386
Area 500: Bioconversion and Upgrading	$53,665,044
Area 600: Wastewater	$55,485,761
Area 700: Lignin	$199,886,681
Area 800: Boiler	$33,165,542
Area 900: Utilities & Storage	$12,696,150
Total Installed Equipment Cost	$501,902,274
Added Direct + Indirect Costs	$460,897,726
(% of TCI)	48%
Total Capital Investment (TCI)	$962,800,000
Installed Equipment Cost/Annual GGE	$17.35
Total Capital Investment/Annual GGE	$33.27
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)	47.8%
From Biomass (Fuel C / Biomass C)	23.3%
BKA Carbon Efficiency from Biomass	3.2%
Maximum Yields (100% of Theoretical)[a]	
Fuel Production (U.S. ton/yr)	128,798
Current Fuel Production (U.S. ton/yr)[b]	88,762
Current Yield (Actual/Theoretical)	68.9%

[a] *Complete conversion of biomass carbohydrates fuel*

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

Manufacturing Costs (cents/GGE fuel product)	
Feedstock + Handling	195.8
Sulfuric Acid	34.6
Caustic	75.8
Sodium Carbonate	38.44
Glucose (enzyme production)	29.5
Hydrogen	0.0
Electricity (import)	108.0
Other Raw Materials	72.8
Catalysts	3.5
Waste Disposal	5.0
Na2SO4 Coproduct	-74.0
BKA coproduct ($0.86/lb)	-137.4
Fixed Costs	84.8
Capital Depreciation	105.4
Average Income Tax	31.7
Average Return on Investment	287.0
Total	860.8

Manufacturing Costs ($/yr)	
Feedstock + Handling	$56,700,000
Sulfuric Acid	$10,000,000
Caustic	$21,900,000
Glucose (enzyme production)	$8,500,000
Hydrogen	$0
Electricity (import)	$31,300,000
Other Raw Materials	$21,100,000
Catalysts	$1,000,000
Waste Disposal	$1,500,000
Na2SO4 Coproduct	-$21,400,000
BKA coproduct ($0.86/lb)	-$39,800,000
Fixed Costs	$24,500,000
Capital Depreciation	$30,500,000
Average Income Tax	$9,200,000
Average Return on Investment	$83,000,000
Total	$238,000,000

Specific Operating Conditions	
Enzyme Loading (mg/g cellulose)	10.0
Net Electricity Import (kWh/GGE)	16.1
Plant Electricity Use (kWh/GGE)	17.9

Appendix B. Life Cycle Inventory (LCI) for 2022 SOT Benchmark Models

BDO Pathway

	2022 SOT (Burn Lignin)	2022 SOT (Convert Lignin – BKA)	
Products	**Production Rate**		
Hydrocarbon fuel	11,942	11,948	kg/h
	126	126	MM kcal/h (LHV)
Coproducts			
Beta-ketoadipate	0	2,645	kg/h
Recovered sodium sulfate salt from WWT	12,642	16,550	kg/h
Export electricity	-	-	kW
Resource Consumption	**Flow Rate (kg/h)**		
Biomass feedstock (20% moisture)	104,167	104,167	
Sulfuric acid, 93%	11,124	12,472	
Caustic (as pure)	2,750	4,550	
Sodium carbonate	7,500	7,500	
Ammonia	1,059	1,960	
Glucose	1,336	1,336	
Corn steep liquor	929	929	
Corn oil	7	7	
Host nutrients	37	37	
Sulfur dioxide	9	9	
Diammonium phosphate	104	104	
Flocculant	433	433	
Toluene solvent makeup	0	0	
Hydrogen	945	948	
Ethanol	0	0	
Boiler chemicals	0	1	
Flue gas desulfurization lime	116	174	
WWT polymer	31	0	
Cooling tower chemicals	1	1	
Makeup water	112,059	144,834	
Natural gas for boiler	0	6,800	
Natural gas for hot oil system	0	0	MMBtu/h
Grid electricity (net import)	29,515	44,353	kW
Waste Streams	**Flow Rate (kg/h)**		
Disposal of ash	4,301	4,398	
Air Emissions	**Flow Rate (kg/h)**		
H_2O	95,114	100,076	
N_2	496,990	429,643	
CO_2	105,430	118,729	
O_2	80,284	33,643	
NO_2	22	37	
SO_2	7	11	
CO	77	66	
CH_4	3	0	

	2022 SOT (Burn Lignin)	2022 SOT (Convert Lignin – BKA)	
Products	**Production Rate**		
Hydrocarbon fuel	10,231	10,212	kg/h
	108	107	MM kcal/h (LHV)
Coproducts			
Beta-ketoadipate	0	2,674	kg/h
Recovered sodium sulfate salt from WWT	12,446	17,430	kg/h
Export electricity	-	-	kW
Resource Consumption	**Flow Rate (kg/h)**		
Biomass feedstock (20% moisture)	104,167	104,167	
Sulfuric acid, 93%	11,124	13,380	
Caustic (as pure)	2,750	5,292	
Sodium carbonate	7,500	7,500	
Ammonia	1,242	2,209	
Glucose	1,336	1,336	
Corn steep liquor	1,276	1,276	
Corn oil	7	7	
Host nutrients	37	37	
Sulfur dioxide	9	9	
Diammonium phosphate	177	177	
Flocculant	418	418	
Toluene solvent makeup	90	90	
Hydrogen	0	0	
Ethanol	0	0	
Boiler chemicals	0	0	
Flue gas desulfurization lime	119	191	
WWT polymer	35	0	
Cooling tower chemicals	3	1	
Makeup water	325,149	254,541	
Natural gas for boiler	0	400	
Natural gas for hot oil system	39	39	MMBtu/h
Grid electricity (net import)	8,697	58,127	kW
Waste Streams	**Flow Rate (kg/h)**		
Disposal of ash	4,306	4,427	
Air Emissions	**Flow Rate (kg/h)**		
H_2O	125,255	92,392	
N_2	479,410	591,298	
CO_2	111,941	108,578	
O_2	74,346	110,301	
NO_2	48	6	
SO_2	8	12	
CO	82	30	
CH_4	3	0	