



Algal Biomass Conversion to Fuels via Combined Algae Processing (CAP): 2020 State of Technology and Future Research

Matthew Wiatrowski and Ryan Davis

National Renewable Energy Laboratory

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Contract No. DE-AC36-08GO28308

Technical Report
NREL/TP-5100-79935
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Suggested Citation

Wiatrowski, Matthew and Ryan Davis. 2021. *Algal Biomass Conversion to Fuels via Combined Algae Processing (CAP): 2020 State of Technology and Future Research*. Golden, CO: National Renewable Energy Laboratory. NREL/TP-5100-79935.
<https://www.nrel.gov/docs/fy21osti/79935.pdf>.

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303-275-3000 • www.nrel.gov

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Acknowledgements

The authors wish to thank the following researchers for their contributions to this work: Lieve Laurens, Eric Knoshaug, Tao Dong, Jake Kruger, Nick Nagle, Yat-Chen Chou, Christopher Kinchin, Bruno Klein, and Zia Abdullah from the National Renewable Energy Laboratory (NREL); Lynn Wendt and Brad Wahlen from Idaho National Laboratory (INL); Phil Pienkos from Polaris Renewables; Steve Mayfield and Marissa Tessman from the University of California San Diego (UCSD)/Algenesi Materials; Haoren Lu from Nexant; and other partners in the Rewiring Algal Carbon Energetics for Renewables (RACER) project (Bioenergy Technologies Office grant). This report provides a high-level overview of research data across key unit operations as utilized in updating NREL's State of Technology (SOT) benchmark models based on inputs furnished from those researchers; however, it is not intended to present an exhaustive summary of all research activities, methods, or data outputs, and we defer to those and others' research works for further context.

List of Acronyms

AD	anaerobic digestion
AFDW	ash-free dry weight
ASU	Arizona State University
AzCATI	Arizona Center for Algae Technology and Innovation
BDO	2,3-butanediol
BETO	Bioenergy Technologies Office
CA	carboxylic acids
CAP	combined algae processing
CUBI	catalytic upgrading of biochemical intermediates (under ChemCatBio consortium)
DEOA	Diethanolamine
DISCOVER	Development of Integrated Screening, Cultivar Optimization, and Verification Research
FA	Florida Algae (test bed site under ATP ³ consortium)
FAME	fatty acid methyl ester
FFA	free fatty acid
FY	fiscal year
GGE	gallon gasoline equivalent
HCSD	high-carbohydrate <i>Scenedesmus</i>
HDO	hydrodeoxygenation
HI	hydroisomerization
HLSD	High-lipid <i>Scenedesmus</i>
INL	Idaho National Laboratory
MBSP	minimum biomass selling price
MFSP	minimum fuel selling price
MOT	mild oxidative treatment
NIPU	non-isocyanate polyurethane
NREL	National Renewable Energy Laboratory
PU	polyurethane
PUFA	poly-unsaturated fatty acid
RACER	Rewiring Algal Carbon Energetics for Renewables
R&D	research and development
SLS	solid-liquid separation
SOT	state of technology
TAG	triacylglyceride
TDI	toluene diisocyanate
TEA	techno-economic analysis
UCSD	University of California, San Diego
USFA	unsaturated fatty acid

Executive Summary

The annual State of Technology (SOT) assessment is an essential activity for platform research conducted under the Bioenergy Technologies Office (BETO). It allows for the impact of research progress (both directly achieved in-house at NREL and furnished by partner organizations) to be quantified in terms of economic improvements in the overall biofuel production process for a particular biomass processing pathway, whether based on terrestrial or algal biomass feedstocks. As such, initial benchmarks can be established for currently demonstrated performance, and progress can be tracked toward out-year goals to ultimately demonstrate economically viable biofuel technologies.

NREL's algae SOT benchmarking efforts focus both on front-end algal biomass production and separately on back-end conversion to fuels through NREL's "combined algae processing" (CAP) pathway. The production model is based on outdoor long-term cultivation data, enabled by comprehensive algal biomass production trials conducted under Development of Integrated Screening, Cultivar Optimization, and Verification Research (DISCOVER) consortium efforts and driven by data furnished by Arizona State University's (ASU's) Arizona Center for Algae Technology and Innovation (AzCATI) test bed site. The CAP model is primarily based on experimental efforts conducted under NREL research and development projects, with some process parameters provided by partner organizations. Assumptions regarding the wet storage of algae use data provided by Idaho National Laboratory (INL), while parts of a newly incorporated polyurethane production process leverage BETO-funded research from collaborators at Algenesi and the University of California, San Diego (UCSD).

This report focuses on back-end conversion of algal biomass through the CAP pathway, highlighting the 2020 updates to minimum fuel selling price (MFSP). Notably, this analysis marks the first time that polyurethane (PU) is included as a value-added coproduct in the SOT case. It is well understood that reaching target MFSPs for algal biofuel production must involve substantial revenue from a high-value coproduct; the inclusion of PU in the SOT represents an important step in making this necessity a reality. Polyols are produced from algal lipids using a one-pot epoxidation and ring-opening reaction, which are then further reacted with an isocyanate cross-linker to produce a flexible polyurethane foam. In recent years, NREL has made significant advancements in the production of a non-isocyanate polyurethane (NIPU) foam, which has the benefit of avoiding toxic and environmentally harmful isocyanates; however, the cost details and commercial scale-up ramifications of a full-scale NIPU facility have yet to be fully understood. Thus, a conventional (isocyanate-based) polyurethane process is reflected as an exemplary approach to inclusion of high-value PU coproducts in a CAP biorefinery, based on inputs furnished from Algenesi/UCSD.

In addition to the inclusion of PU in the CAP process, the upstream biomass costs (minimum biomass selling price [MBSP]), yields, and seasonal variability from the upstream cultivation SOT model were also incorporated into downstream Aspen Plus CAP models, reflecting experimental data from NREL CAP research and development activities. Other advancements included in the fiscal year (FY) 2020 SOT include increased sugar yields from dilute acid pretreatment (83% versus prior yields of 74%) and improvements in seasonal storage.

Beyond the changes outlined above, the CAP SOT model inputs are consistent with prior SOTs from recent years. These inputs include values of 95% fermentable sugar recoveries across a membrane solids removal step and 96% lipid extraction recovery from biomass solids. The clarified sugars achieved 92% conversion of glucose and mannose to carboxylic acids during fermentation over a productivity of 0.3 g/L-hr yielding 0.41 g acids/g available sugars (based on data from NREL algae platform research), or 89% conversion of glucose and mannose to upgradeable intermediate (2,3-butanediol [BDO] and acetoin) over a 56-hour batch time, yielding 0.33 g BDO/g sugars (based on data from NREL algae research conducted under the Rewiring Algal Carbon Energetics for Renewables [RACER] project grant). Maintaining those same fractional conversions and other operational parameters coupled with the updated 2020 SOT MBSP value of \$682/ton (based on ASU evaporation rates), the 2020 MFSP translates to \$6.12/gallon gasoline equivalent (GGE) and \$6.50/GGE for the acids and BDO fermentation pathways, respectively. Alternatively, the 2020 MBSP value associated with Florida Algae (FA) evaporation rates at \$603/ton ash-free dry weight (AFDW) would reduce the MFSP to \$4.94/GGE and \$5.33/GGE for the acids and BDO cases, respectively.

Relative to the 2019 SOT case, this indicates an improvement of \$4.3–\$4.4/GGE (roughly 40%–45%) for both the acids and BDO pathways. In all cases, the addition of full pond liners in the upstream biomass farm models would increase SOT fuel costs by approximately \$2.5/GGE relative to the above values based on minimally lined ponds. As in prior SOTs, these results are all based on an assumed biomass composition consistent with NREL’s high-carbohydrate *Scenedesmus* (HCSD) composition targets.

The resulting total fuel yields were modeled as 63.0 GGE/ton and 62.9 GGE/ton AFDW for the acids and BDO pathways, respectively, translating to 1,685 and 1,682 GGE/acre-year when including upstream cultivation productivity and seasonal biomass storage losses (based on wet seasonal storage reflective of HCSD biomass compositions). These yields mark a decrease compared to prior years, due to a partial diversion of lipids to PU rather than fuels. Finally, this milestone reports on key process sustainability indicators for the CAP conversion stage, including mass and carbon yields to fuels and coproducts, freshwater consumption, and facility power balances/natural gas demands. In keeping with recent BETO guidance, formal life cycle assessment sustainability metrics such as greenhouse gas emissions or fossil energy consumption are not calculated here, but will be deferred to Argonne National Laboratory.

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Introduction

The National Renewable Energy Laboratory (NREL) develops and maintains techno-economic models that simulate the technical and economic aspects of conceptual biorefinery conversion pathways to biofuels and bioproducts, focused on both terrestrial and algal biomass processing routes. For a particular set of process parameters, material and energy balance and flow rate information is generated using Aspen Plus simulation software [1], for a given facility size or biomass throughput rate. 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) or minimum biomass selling price (MBSP) required to obtain a net present value of zero for a 10% internal rate of return is determined. The result is a techno-economic model that reasonably estimates an “ n^{th} -plant” production cost for this pre-commercial process.

Over recent years, NREL has published a number of reports for both the production of algal biomass and the conversion of algae to fuels via the “combined algae processing” (CAP) pathway [2–4], all of which focus on achieving a modeled MFSP of \$2.50/gasoline gallon equivalent (GGE) from algal biomass. Combined analysis from the 2014 and 2016 reports [3, 4], which focus primarily on the production of algal fuels (fermenting sugars to ethanol and upgrading lipids to diesel-range blendstocks), finds an MFSP of \$5.90/GGE (2014\$) when considering out-year targets. Even considering substantial improvements around biomass cultivation costs (with MBSP goals near \$500/ton, representing the largest contributor to overall fuel cost), this represents a roughly sevenfold increase over terrestrial biomass cost goals [5]. At even high fuel yield targets of 100 GGE/ton, as can be achieved from algal biomass conversion pathways, this translates to a minimum MFSP of \$5/GGE tied to feedstock cost alone. Thus, it has become increasingly clear that additional biorefinery revenue will be necessary in order to offset feedstock and conversion processing costs to reduce MFSPs. Accordingly, recent iterations of the CAP process have begun to consider the inclusion of value-added coproducts to ultimately meet Bioenergy Technologies Office (BETO) targets of \$2.5/GGE by 2030 [6].

In light of this importance for non-fuel coproducts to be produced alongside fuels in order to drive down MFSPs in the future, various coproducts have been considered for inclusion in the CAP pathway (including succinic acid, surfactants, plastics, and polyols/polyurethanes). Polyurethane (PU) foam, producible from the unsaturated fatty acids found in algae, was identified as a leading candidate to supplement the revenue required to offset feedstock costs due to relatively high selling prices and market volumes. However, the conventional method of polyurethane production involves the reaction of isocyanates, which are considered deleterious to health and the environment. Accordingly, NREL research and development (R&D) began to investigate a novel route to polyurethane circumventing the need for isocyanates. Thus far, this research has shown promising results, successfully demonstrating proof of concept for a non-isocyanate polyurethane (NIPU) foam produced from algal lipids using diamine cross-linkers [7]; however, the research is still considered to be in early stages with higher uncertainties regarding design, cost, and scale-up implications for TEA modeling purposes for this pathway to be considered for inclusion in the SOT at present. Considering that conventional (isocyanate-based) polyurethane is outside the NREL R&D scope, it was considered only as a future target case within the 2018 and 2019 SOTs, with corresponding SOT cases utilizing lipids for fuel

production exclusively [8]. However, the costs and technical parameters associated with the production of conventional polyurethane from algal lipids have been further developed and refined as part of a recently published CAP conceptual design update [2], highlighting a key role in achieving a projected MFSP of \$2.56/GGE for the conceptual basis of a new potential CAP process considering out-year targets. Although conventional PU remains outside of the NREL R&D scope, the technology readiness level is sufficiently advanced to warrant inclusion into an SOT analysis, given appropriate access to data with successful production of algal-based foams demonstrated in industry [9]. Accordingly, data for the production of conventional PU from algal lipids was obtained from BETO-funded research via industry and academic collaborators Algenesis and the University of California, San Diego (UCSD) for inclusion in the present SOT to demonstrate proof of concept for incorporation of a PU coproduct opportunity into a CAP biorefinery schematic. This inclusion marks an important step ultimately necessary to meet BETO targets of \$2.50/GGE by 2030.

We emphasize that the present SOT analysis and the resultant MBSP and MFSP values carry some uncertainty related to the assumptions and estimates made for capital and raw material costs. Without a detailed understanding of the underlying basis, the absolute computed selling price has limited relevance. 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 because no commercial algal biofuel facility exists today (e.g., growing algal biomass for purposes of producing fuels at commercial scale), and because the SOT performance results documented here are based solely on NREL and partner (DISCOVER consortium, Idaho National Laboratory [INL], and UCSD) data and do not necessarily represent a broader picture of all performers within and beyond BETO’s portfolio.

Discussion of Relevant Inputs Used in the SOT

The base case CAP configuration as reflected in NREL's fiscal year (FY) 2020 SOT is shown in Figure 1. This configuration reflects a similar process design as shown in prior recent SOT reports; the only difference is that here, a portion of the lipids are used for the production of a polyurethane coproduct, whereas prior configurations diverted all lipids to fuel production [8, 10]. This inclusion of a high-value coproduct (in this case polyurethane) is a key enabling factor to achieving \$2.5/GGE MFSP goals by 2030 [6, 10].

In summary, the process approach utilizes diversion of peak seasonal biomass capacity from upstream cultivation in excess of the annual average feed rate to a wet anaerobic storage process, and pulling from storage during low-production seasons below the average (with wet storage performance data furnished by partners at INL [11]). The material is delivered from cultivation after dewatering to 20 wt% solids ash-free dry weight (AFDW). Following storage as applicable, the biomass is routed to dilute acid pretreatment, traditionally used to hydrolyze carbohydrates to monomeric sugars and enable effective downstream lipid extraction. In the present SOT, more recent acid pretreatment yields were incorporated, reflecting biomass samples (*Scenedesmus acutus* LRB-AP-0401) derived from INL's storage study achieving 83% overall combined sugar yields (84% glucose/70% mannose for fresh algae and 81% glucose/92% mannose for stored algae) when processed through NREL's ZipperClave pretreatment reactor at standard conditions [12]. This represents an improvement over historical SOT data previously reflected at 74% combined yields from earlier work.

The pretreated hydrolysate slurry is processed through solid/liquid separation using a vacuum filter press, with the solids routed to extraction and the liquor routed to sugar fermentation. The basis SOT schematic reflects two fuel fermentation pathways based on similar focus areas under the Biochemical Conversion Platform, namely fermentation to carboxylic acid or 2,3-butanediol (BDO) intermediates, in either case subsequently upgrading the given intermediate to final hydrocarbon fuel products through a series of catalytic steps. Both sugar fermentation pathways considered here are maintained to be consistent with the FY 2018 and FY 2019 SOTs, aside from small modifications made to reflect improved convertibility of fermentation intermediate derivatives.

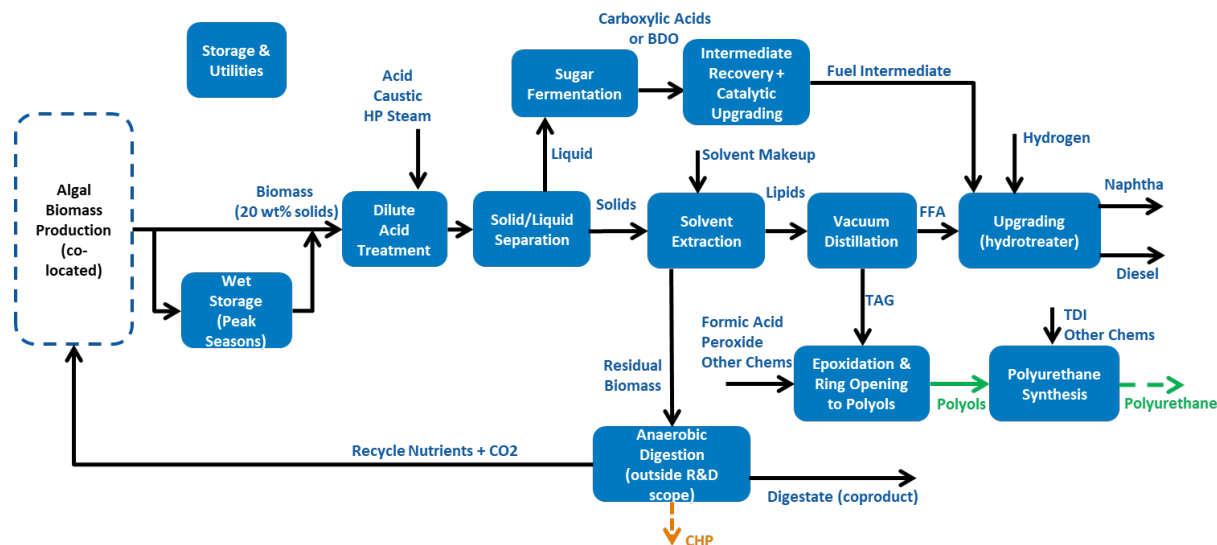


Figure 1. Schematic diagram of CAP configuration for the FY 2020 SOT

The solids product from upstream solid/liquid separation is routed to lipid extraction across a series of three mixing/phase separation steps in series, each utilizing a nonpolar (hexane or light naphtha) solvent with a polar (ethanol) co-solvent. Both the extract and raffinate phases are routed to distillation columns for recovery and recycle of the respective solvents. The raffinate product, enriched in protein after ethanol solvent recovery, is routed to anaerobic digestion (AD) to produce biogas for heat and power benefits as well as enabling recycle of N/P nutrients back to cultivation. The remaining lipids undergo a three-step purification process to remove impurities, followed by a vacuum distillation step to yield triacylglycerides (TAGs) and free fatty acids (FFAs). The FFA portion is routed to hydrotreating for production of hydrocarbon fuels (consisting of a combined hydrodeoxygenation/hydroisomerization [HDO/HI] step), while the TAG portion is used to produce polyurethane. Process parameters for the pretreatment, sugar fermentation, and lipid extraction and upgrading sections are shown in Table 1.

Table 1. Process Conditions and Conversions Observed from Experimental CAP Data, Utilized for FY 2020 SOT [13–16]. Italicized lines represent modeling assumptions, outside experimental scope. Polyol/polyurethane production details are presented separately in Table 2.

Pretreatment	Value		Experimental Notes
Solids loading (wt%)	20% ^a		<ul style="list-style-type: none">Pretreatment data reflect new NREL experimental work done under CPR project based on INL seasonal storage materialSLS vacuum membrane based on FY 2017 data
Acid loading (wt% vs. feed liquor)	2%		
Fermentable sugar release	83%		
Carbs to degradation products	1.5%		
Hydrolsate solid-liquid separation (SLS)	Yes (vacuum belt filter with flocculant)		
Sugar loss in solid-liquid separation	5%		
Lipid loss in solid-liquid separation	0.5%		
SLS flocculent loading (g/kg IS)	10		
SLS membrane capacity (kg IS/m ² -h)	30		
Sugar Fermentation	Acids	BDO	<ul style="list-style-type: none">Acids data based on NREL algae platform R&D in FY 2018; BDO data based on inputs from NREL researchers under FY 2018 RACER project fermentation work on <i>Desmodesmus</i> C046
Fermentation productivity (g/L-hr)	0.3	56-hour batch	
<i>Sugar diversion to organism seed growth</i>	10% ^b	10% ^b	
Glucose utilization to product	92% ^c	89% ^{c, d}	
Mannose utilization to product	92% ^c	89% ^{c, d}	
Glycerol utilization to product	92% ^c	0% ^{c, d}	
Butyric acid yield (g/g total available sugars)	0.39	N/A	
Acetic acid yield (g/g total available sugars)	0.10	N/A	
BDO yield (g/g total available sugars)	N/A	0.33	
Acetoin yield (g/g total available sugars)	N/A	0.09	
Catalytic upgrading carbon efficiency (HDO feed vs. recovered intermediate) ^e	83%	98%	
Lipid Extraction + Upgrading			<ul style="list-style-type: none">Extraction yields based on high-carbohydrate <i>Scenedesmus</i> (HCSD) biomass, FY 2018 data with light naphtha solventHydrotreating (HDO+HI) yields based on HCSD-extracted lipids, maintaining FY 2017 data for one-step HDO + HI upgrading
Extraction configuration	3-stage CSTR + centrifugation with 2 solvents		
Solvent loading (nonpolar: EtOH: dry biomass, wt)	2.7:1.1:1 g/g/g		
CSTR extraction residence time (min)	15		
Convertible lipid extraction yield per step	74%, 65.4%, 55.6%		
Total convertible lipid extraction yield	96.0%		
Non-sterol lipid impurity partition to extract	<11.5%		
Hydrotreating conditions	707°F, 435 psig, ~5,900 scf/bbl H ₂ feed ratio		
Catalyst details	1% Pt/SAPO-11, 1 h ⁻¹ WHSV		
Hydrotreating renewable diesel blend-stock yield (wt% of oil feed) ^f	62.1%		
Hydrotreating naphtha yield (wt% of oil feed) ^f	21.8% ^g		
Hydrotreating H ₂ consumption (wt% of oil feed)	2.23% ^h		

^a Experimental work based on 18%–25% solids, adjusted here to 20% solids for consistency with previously published modeling framework; pretreatment performance is expected to remain unchanged at this value (unpublished data)

^b Values were not determined here as part of the scope of experimental work; set consistent with previously documented models [3]

^c Does not include sugar diversions to biomass seed growth assumed in the model

^d Includes BDO and acetoin

^e Catalytic upgrading of fermentation intermediates to final hydrocarbon fuels is outside R&D scope; set consistently with 2017 *Algae Harmonization Study* for acids case [6] and Biochemical Platform FY 2018 SOT data for BDO case. Value represents upgrading yields to the final fuel finishing (hydrotreating) reactor feed.

^f Hydrotreating yields are based on adjusting original experimental data [14] to achieve 100% mass closure, based on lipid hydrotreating alone (not including co-processed BDO/acids intermediate products)

^g Includes light gas correction, estimated separately via mass and element closure to 100%; based on lipids alone

^h H₂ consumption set in model to close elemental H balance; experimental H₂ consumption measured was lower; based on lipids alone.

The polyurethane production process, shown below in Figure 2, consists of a one-pot epoxidation and ring-opening reaction to polyols, followed by polymerization with toluene diisocyanate to produce polyurethane foam. This “conventional” polyurethane process, most recently updated as outlined in the 2019 CAP Update Technical Report referenced above [2], uses information furnished from industry databases and engineering subcontractors for the production of polyurethane from algae- or plant-based lipids. In the present SOT assessment, the polyol production portion of the process has been further updated to reflect inputs obtained from industry collaborators Algenesis and UCSD, under the umbrella of BETO-supported research in this space. Recent experimental work at NREL has begun investigating a more novel route to PU products that may offer several benefits over the traditional route described above, primarily avoidance of toxic and environmentally harmful isocyanate cross-linkers [17, 18]. The NIPU route maintains the initial epoxidation step, but rather than epoxide ring opening to polyols, the ring is reacted with CO₂, forming a carbonate group [7, 19]. These carbonate groups may react with diamine cross-linkers to form NIPU end products, potentially enabling a fully renewable PU process given that the diamines could be derived from the algal biomass. While this work has yielded promising results over recent months, the NIPU process has not yet been fully evaluated through TEA modeling and thus is not yet ready for incorporation in the current CAP SOT update, primarily given uncertainties related to design and costs upon scale-up to commercial levels and resultant market values of the NIPU material. Recent work (manuscript submitted) has investigated the production of NIPU foam from various sources of triglycerides (including linseed oil and algal oil), with preliminary TEA implications also considered. In FY 2021, this analysis will be integrated with the CAP modeling framework to evaluate its impact on algae biorefinery economics. However, at present, the conventional isocyanate route is included here as an exemplary reflection of this coproduct opportunity in the CAP process.

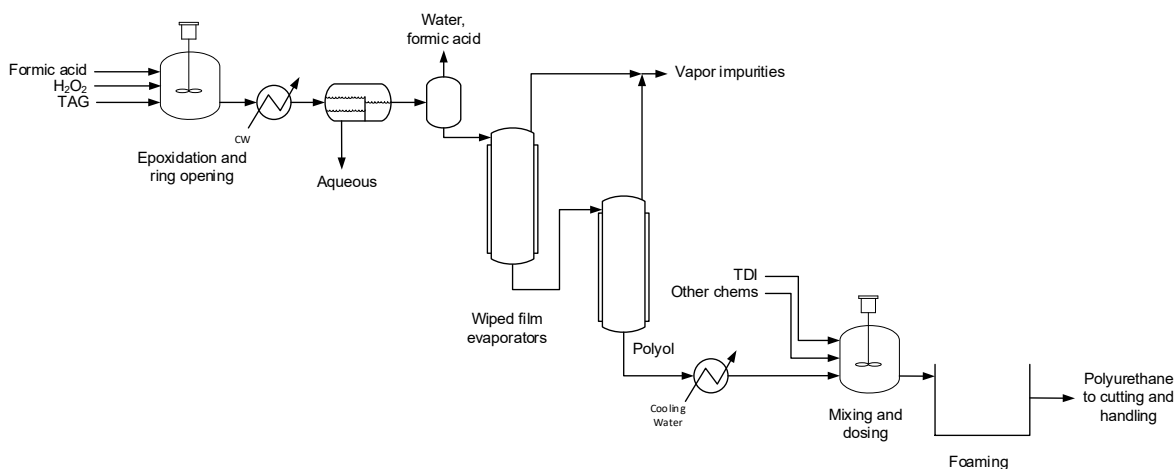


Figure 2. Process flow diagram of the polyol/polyurethane production train for the FY 2020 SOT

The modeled isocyanate polyurethane production process uses inputs from Algenesis/UCSD as well as an engineering subcontractor to NREL (Nexant) and literature; major process parameters are shown in Table 2. Algal TAGs undergo epoxidation and ring-opening reactions to yield polyols. Recent work at UCSD [20] as well as elsewhere [21] has shown success in converting

TAG to polyols in one vessel, executing both reactions simultaneously and minimizing equipment costs. While this approach was used in the CAP 2019 Technical Report, it has been updated here to more optimized reactants and conditions reflective of demonstrated process data. Peroxide and formic acid (rather than the acetic acid specified in the CAP 2019 report) react with TAG to epoxidize the double bonds present. The epoxide rings are then opened by formic acid (forming one hydroxyl group per double bond) or water (forming two hydroxyl groups per double bond). Water is present from the peroxide (fed as an aqueous 70% solution) and is also produced *in situ* from the reaction of peroxide. The ratio of rings opened by acid to water can change the final properties of the polyurethane, since the degree of cross-linking is directly related to hydroxyl number (a function of the average number of double bonds per unit mass of polyol). In this analysis, we have assumed a 1:1 ratio of the two ring-opening reactions.

Following epoxidation and ring opening, the design of the polyurethane production process is consistent with the 2019 CAP report. The polyol is sent to two wiped film evaporators in series, each at mild vacuum and temperatures up to 140°C and 260°C, respectively. These evaporators remove high-boiling impurities which can cause odors in the final product. The finished polyol product from the second evaporator is then cooled and sent to the foam production line. This consists of four sections: raw material tank farm, mixing and dosing section, foaming section, and the cutting and handling section. The final PU product is sold at a fixed price of \$2.04/lb (2016-dollars), representing a recent 5-year average price for commodity flexible PU foam [2].

Note that in the foaming section, the cross-linking component TDI is added in the theoretical stoichiometric amount to react with the hydroxyl groups (0.5 moles of TDI per mole of hydroxyl groups). The ratio of the actual isocyanate used relative to the theoretical amount is commonly referred to as the isocyanate index; thus, we assume an isocyanate index of 1.0. Our prior analysis assumed a higher isocyanate index of 1.34 based on subcontractor input [2]; however, it is believed that this was an overestimate and did not correctly take into account the average functionality of the polyols. While it is possible that an isocyanate index between these two numbers would be appropriate for this process, a conservative estimate of 1.0 is assumed. Higher isocyanate indexes will further benefit process economics, since TDI directly contributes to polyurethane yields.

Table 2. Process Inputs for Polyurethane Production

Parameter	Specification	Basis
Epoxidation and ring-opening		
Temperature	75°C	[20]
Pressure	1 atm	[20]
Residence time	6 hours	[20]
H ₂ O ₂	1.5x double bonds	50% stoichiometric excess
Formic acid	Equimolar with double bonds	[20]
Power	0.54 MWh/ton polyol	Input from Nexant [2]
Cooling water	220 w/w polyol	Input from Nexant [2]
Low-pressure steam	0.02 w/w polyol	Input from Nexant [2]
Nitrogen	0.02 w/w polyol	Input from Nexant [2]
Other chemicals	\$46.70/ton polyol	Input from Nexant [2]
Polyurethane production		
TDI ^a	0.5 mole/mole hydroxyl group	Stoichiometric
Water	0.0281 w/w polyol	Input from Nexant [2]
DEOA ^b	0.0026 w/w polyol	Input from Nexant [2]
Surfactant	0.0049 w/w polyol	Input from Nexant [2]
Power	0.004 w/w polyol	Input from Nexant [2]

^a Toluene diisocyanate

^b Diethanolamine

In keeping with prior FY 2018–2019 CAP SOTs, both sugar fermentation pathways reflected in the recent CAP SOT configurations are again maintained here via acid and BDO intermediates. While no notable efforts or improvements were made to either case under FY20 Algae Platform activities due to experimental focus on alternative processes (discussed below), ongoing work under the Biochemical Conversion Platform has demonstrated continued improvements for both fermentation pathways over recent SOTs [22]. Namely, the carboxylic acid pathway has demonstrated over 95% conversion of glucose to product with minimal diversion of sugars to acetic acid (1:50 ratio of acetic vs. butyric acid production) and a doubling of productivity from 0.3 to 0.6 g/L-hr using *Clostridium tyrobutyricum*, also based on a physically integrated fermentation-pertraction setup with *in situ* removal of acids at a 98.4% recovery rate of butyric acid. The BDO pathway has also demonstrated nearly 100% utilization of glucose with 90% overall theoretical yield to BDO within 48 hours (roughly 30% improvement over FY 2018 productivity) and minimal acetoin byproduct, using an engineered strain of *Zymomonas mobilis*. Downstream steps under ChemCatBio (catalytic upgrading of biochemical intermediates [CUBI])-supported efforts also demonstrated nearly 100% conversion for all catalytic upgrading steps within the scope of experimental work (excepting ketone condensation for the acids pathway, demonstrated at 40% per-pass conversion or 92% overall net conversion of ketones to condensation products). The present SOT update also reflects improvements for the BDO pathway in co-utilization of acetoin (produced as a byproduct from BDO fermentation) achieved over recent years under CUBI, and the acid pathway corrects for a minor slipstream loss of an intermediate formed during acid upgrading operations (leading to increased fuel yields across catalytic upgrading for both pathways).

In all, assuming similar performance levels could also be achieved here under the algae CAP process (likely to be possible barring any differences with mannose, which is present for algae but not for corn stover as utilized in the biochemical platform; although work under the Rewiring Algal Carbon Energetics for Renewables [RACER] project has resulted in an engineered *Zymomonas* strain capable of utilizing mannose on par with glucose), this would largely support achievement of final future performance targets for all fermentation and catalytic upgrading steps, with lipid extraction also having already exceeded final targets. This would leave only pretreatment for future improvement in the prior CAP approaches, in addition to any further advancements on polyurethane or other coproducts. Given that conventional polyurethane production is a generally mature technology (though less mature in terms of using plant- or algae-based lipids), significant further advancements to this particular CAP configuration are unlikely. However, integration of NIPU into future SOTs shows potential for process improvements for this more novel “green” chemistry route, while potentially maintaining a similar production cost as compared to conventional polyurethane.

In addition to the changes to the CAP process configuration and process parameters discussed above, updated FY 2020 cultivation yields, seasonal flows, and biomass costs (MBSP) upstream are also considered. All pertinent details for those parameters are summarized in the accompanying FY 2020 algal biomass SOT report; in summary, FY 2020 algae farm MBSPs were estimated at \$683/ton or \$603/ton AFDW for the Arizona State University (ASU) vs. Florida Algae (FA) evaporation scenarios, respectively (unlined ponds, increasing to \$853/ton or \$772/ton for fully lined ponds, respectively). This was tied to a 16% improvement in annual cultivation productivity (18.4 g/m²/day, over the FY 2019 basis of 15.9 g/m²/day) and a lower seasonal variability between summer vs. winter cultivation seasons (3.8:1, compared to 4.2:1 in FY 2019). Beyond a lower biomass feedstock cost, the FY 2020 SOT update also reflects the associated higher throughputs through the CAP processing facility (roughly 134,000 tons/year versus 116,000 tons/year in FY 2019 tied to a fixed 5,000-acre algae farm facility), incurring economy-of-scale improvements for CAP processing.

Consistent with prior SOTs, variability in biomass delivery rates from upstream seasonal cultivation is mitigated by diverting excess peak biomass capacity to a wet anaerobic storage process, to be blended with biomass from cultivation during low production seasons, targeting a fixed throughput rate through the CAP facility all year. The wet storage concept and associated data is based on collaborations with partners at INL, who have been coordinating work on this subject over recent years [11]. In the FY 2020 SOT, the details around the storage degradation losses and compositional shifts are updated according to the most recent data from INL. This updated basis shows a notable improvement in overall degradation loss (13%, compared to a 23% loss previously), as well as an adjustment in the compositional changes and acid production in the stored biomass (personal communication, Brad Wahlen [INL], November 2020). The fresh and stored biomass compositions are summarized in Table 3, based on inputs from INL extrapolated to the same HCSD strain basis assumed here. The resulting raw seasonal and post-storage biomass flowrates are depicted in Figure 3. At the 3.8:1 seasonal variability from cultivation, roughly 20% of total annual biomass production must be sent to seasonal storage, which—coupled with the 13% storage degradation losses—translates to a minor 2.6% overall loss of annual biomass feed to the CAP facility. This is a substantial improvement compared to the FY 2019 SOT, which corresponded to a 6% overall loss of annual biomass due to storage degradation. The acid degradation products are ultimately relegated to AD, with the exception of a small amount of acetic acid which gets converted in the acids pathway.

Table 3. Input Compositions to CAP Models Before and After Wet Storage Losses, Based on Raw HCSD Composition as Well as Adjustments Applied to the HCSD Baseline to Reflect Degradation Losses as Measured by INL [11], (personal communication, Brad Wahlen [INL], November 2020)

	Raw Algae	Wet Storage Algae
Solids Content (wt%)	20	20
Algae Composition (wt%)		
Fermentable carbohydrates	47.8	45.5
Protein	13.2	13.2
TAG	14.5	15.0
FFA	13.0	13.4
Glycerol	1.5	1.5
Ash	2.4	2.4
Non-fermentable carbohydrates	3.2	3.0
Sterol	1.8	2.4
Non-fuel polar lipid impurities	1.0	1.4
Cell mass	1.6	2.2
Sum	100.0	100.0
Whole algal biomass intact after storage (kg)	1.0	0.868
Acid produced per kg of whole algae (after storage)		
Succinic acid, kg		0.037
Lactic acid, kg		0.052
Acetic acid, kg		0.003
Propionic acid, kg		0.006

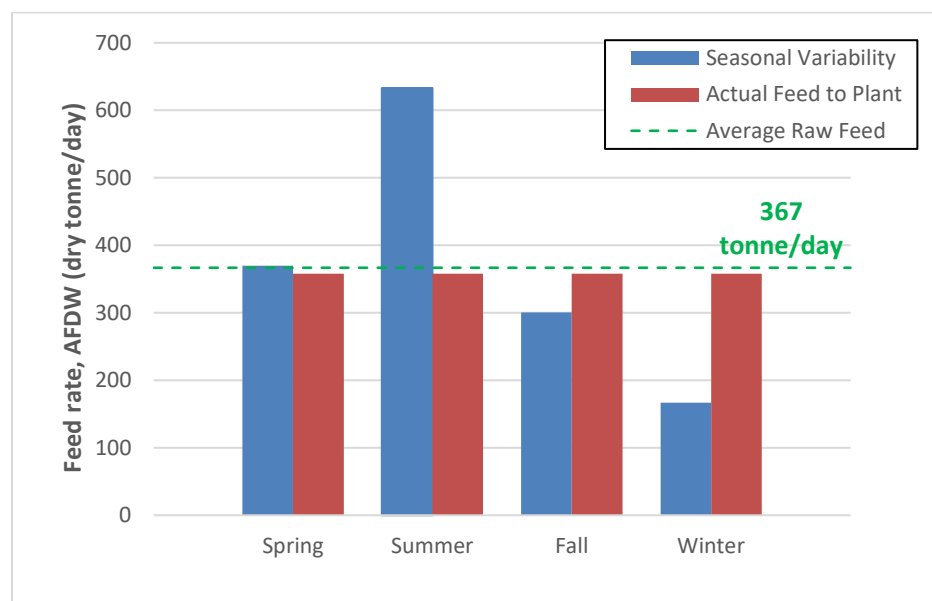


Figure 3. Seasonal and annual average feed rates to conversion facility (AFDW basis, FA evaporation scenario)

SOT basis assumes seasonal storage scenario represented by red bars (lower than annual average of blue bars due to seasonal storage losses)

Discussion of Alternative Processes

In FY 2019, NREL experimental efforts were conducted with a high-ash, halotolerant algal species to demonstrate conversion through the CAP process depicted in Figure 1 for saltwater algae (*Scenedesmus* IITRIND2) [23]. Although prior work had been conducted on non-freshwater algae species of various salinities with good results, this particular IITRIND2 species was seen to exhibit high recalcitrance with low carbohydrate hydrolysis across pretreatment, generally below 20% monomeric sugar yield across a range of temperatures and acid loadings. This was hypothesized to be due to elevated protein and ash, rendering the biomass more resistant to acid pretreatment, likely with ash incurring a buffering effect to neutralize the acid. Such recalcitrance was also observed in other (but not all) saline strains, suggesting a strain-dependent effect. In light of such low sugar yields, the researchers opted not to pursue further downstream fermentation on this material given that it would not have led to an improvement over previous SOT results (historically based on 74% pretreatment sugar yields demonstrated previously). Rather, the experimental work pivoted to a new CAP approach that had begun to be investigated as a means to bypass the dependence on acid pretreatment and high sugar yields for fermentation, while making use of both carbohydrates and protein (soluble or insoluble), thereby also potentially relaxing the dependence on biomass composition that had historically been affiliated with the CAP pathway.

Briefly, the envisioned process for such an alternative CAP approach is summarized as follows [2, 24]: Following diversion of dewatered biomass to wet seasonal storage as necessary (noted above), the biomass would undergo rapid flash hydrolysis pretreatment to maintain good lipid extraction, albeit without requiring high monomeric sugar yields and thus negating dilute acid pretreatment. The whole slurry may then be routed to lipid extraction following a similar extraction and lipid upgrading sequence as before. The raffinate (containing both carbohydrates and protein) would then be processed through mild oxidative treatment (MOT), employing an oxidant (i.e., oxygen) at moderate temperature and pressure to convert carbohydrates and protein into carboxylic acids. The MOT product, primarily a mixture of mono- and di-carboxylic acids, may be routed to filtration and ion exchange, capturing liberated N and P components for recycle to cultivation, followed by catalytic upgrading through ketonization (forming ketones), condensation (forming oxygenated longer-chain molecules), and HDO (forming finished hydrocarbon fuel components).

While this approach possesses the potential for enabling high fuel yields and, if desired, simultaneous co-production of polyols/polyurethanes [2], some new steps are still in early stages of conceptual development and more remains to be understood moving forward. Namely, preliminary efforts on MOT upgrading have highlighted an important link between MOT yields and oxygen access to the substrate, with favorable yields initially observed under significantly more dilute substrate conditions of 20 g/L (2 wt% solids). This concentration level (2 wt% solids) is not practical for an integrated commercial process (ideally in the 15%–20% range) given both significant throughput volumes requiring very large reactor sizes, as well as significant heating demands to raise the feed temperature to reactor conditions. Though increased conversions of solids have been observed at higher oxygen pressures, the results for conversion of solids have thus far been shown to be ultimately cost-prohibitive. Additional modifications were tested to attempt to increase conversions and yields, including the use of catalysts

(including RuOx/SiO₂ and CuO) and alternate oxidants (H₂O₂). However, these experiments showed minimal measurable benefits. Accordingly, the R&D approach shifted to focus more on MOT of the extracted liquor, which would contain solubilized proteins (in the form of amino acids and polypeptides) and carbohydrates (in the form of monomeric and oligomeric sugars). This approach, when used at a sufficient oxygen pressure (50 bar), has shown promising conversions and yields that are more consistent with what would be required to meet TEA targets. However, this conversion strategy has yet to prove more effective than the BDO and carboxylic fermentation pathways reflected in this report. Moreover, the resultant concentrations and species of acid products from MOT translated into new product species that had not been initially expected from ketonization and condensation, with preliminary data established for those operations to date based on mock acid substrates.

For the above reasons, the new CAP processing configuration approach described above is still deemed to be too premature and not yet optimized for commercial practicality to be ready for use as a formal FY 2020 SOT benchmark. Moving forward, CAP R&D will focus on driving more carbon to the liquor during pretreatment, enabling higher fuel or coproduct yields from the liquor upgrading route. In addition to MOT, which has shown promise as an operation for enabling nutrient recovery, alternate fermentation routes will be investigated, including fermentation to lactic acid and lipids, either of which could play a role in a route to coproducts or fuels. Simultaneously, additional focus will be directed to the valorization of solid residue, with coproduct considerations including use of a co-feed for synthesis of bioplastics, conversion to graphene, or sale as an animal/fish feed. Finally, further experimental work will be conducted across ketonization, condensation, and HDO to further quantify product species and elemental balances across each step based on an integrated process, starting with acids produced in MOT, as well as others such as lactic acid.

Results

TEA Results

The updates discussed above (including the addition of PU co-production, improved acid pretreatment and wet storage performance, and improved biomass flowrates and MBSP costs from the upstream biomass production model) resulted in substantial improvements in overall MFSPs for the FY 2020 SOT. These results are summarized below in Figure 4 for the present FY 2020 SOT across both the acids and BDO fermentation pathways, and for both the ASU and FA evaporation rate assumptions under upstream biomass cultivation; analogous FY 2019 results are also shown for comparison. The results of this analysis indicate an **FY 2020 SOT MFSP of \$6.12/GGE (acids pathway) or \$6.50/GGE (BDO pathway) for the ASU evaporation MBSP basis, or \$4.94/GGE and \$5.33/GGE (acids versus BDO) for the FA evaporation basis (all results in 2016\$)**. Compared to the FY 2019 SOT at \$10.53–\$10.91/GGE for ASU evaporation or \$9.50–\$9.88/GGE for FA evaporation (acids vs. BDO pathways, respectively), this represents an overall MFSP reduction of 40%–48% (\$4.3–\$4.6/GGE). While all of the discussed changes had a positive impact on MFSP, a large portion of this improvement (approximately 75%) can be attributed to the addition of the polyurethane coproduct, which trades a moderate loss of fuel yield for a substantial boost in revenue, due to the comparatively higher value of polyurethane as compared to fuel, based on a fixed polyurethane coproduct credit of \$2.04/lb. Updated MBSPs, tied to improved cultivation productivity, also account for a sizeable portion (approximately 19%) of the year-over-year improvement.

As is noted above and consistent with prior SOTs, these values (for both MBSPs and MFSPs) are all based on the assertion of a fixed algal biomass composition consistent with NREL's HCSD future target projections (i.e., asserting an early stage of nutrient depletion with reduced protein content [13%], mid-level FAME lipid content [26%], and high carbohydrate content [48%]) [4, 10]. A sensitivity case that considered the conversion of the actual harvested biomass composition was also investigated. The harvested composition, which can be found in the accompanying 2020 algal biomass (Algae Farm) SOT report, contains considerably lower carbohydrate (9%) and FAME lipid (9%) content, with corresponding increased protein content (45%). The conversion of this biomass (at an increased MBSP of \$707/ton) within the current CAP process would result in an MFSP of \$38.67/GGE (acids pathway) or \$39.76/GGE (BDO pathway) for the FA evaporation basis. However, it should be stressed that the process design investigated here is not optimized for a high-protein biomass, with protein relegated to the production of biogas via AD, thus this high-protein composition is not a practical match for the current CAP configurations reflected here, and accordingly would not be run through these configurations in a realistic setting. These SOT results would show considerable improvement for an alternative process design optimized for the high-protein biomass.

Between the two fermentation pathways, the acids pathway SOT continues to reflect a slightly lower MFSP than the BDO pathway, driven by comparable yields and operating costs but 7% lower total capital costs (primarily reflecting lower fermentation and upgrading costs, with aqueous BDO upgrading particularly costly at the low 7.3% BDO concentration levels observed in the present SOT). Given further improvements in BDO fermentation yields and use of more concentrated sugars (i.e., increased pretreatment sugar yields or higher sugar concentrations

targeted through evaporation), the MFSP difference between the two fermentation pathways could reduce further.



Figure 4. TEA results for 2019–2020 SOTs across both fermentation pathways (acids vs. BDO) and cultivation evaporation scenarios (ASU vs. FA evaporation MBSP)

Alternative MFSPs assuming fully lined ponds are shown in parentheses (LP = lined ponds)

Figure 5 provides the same MFSP cost breakdowns for the SOT cases as shown in Figure 4, but formatted for simplicity reflecting only the FA evaporation cases, and also including example future projection scenarios for 2025 and 2030 reflecting additional process improvements for algae cultivation and conversion. The future scenarios assume continued improvement in CAP process parameters if this CAP process configuration were to be further pursued (instead of or alongside the “new” CAP configuration discussed earlier), and further improvements in biomass cultivation performance (discussed in the accompanying algal biomass SOT report). Specific process parameters used for each case are shown in Table 4; target improvements considered include advancements in cultivation, pretreatment, and sugar fermentation.

For simplicity, the process parameter targets associated with conversion are kept consistent between the 2025 and 2030 cases; in contrast, cultivation targets are adjusted to show incremental process. While strictly intended to serve as *examples*, the 2025 case reflects an interim biomass yield of 29.4 ton/acre-yr (20 g/m²/day at 330 days/year) [8]. The feedstock cost associated with these parameters is virtually equivalent to the cost for the FY 2020 SOT; therefore, improvements between the FY 2020 SOT and the 2025 target cases would largely imply moving toward achievement of the targeted biomass compositions during cultivation, coupled with targeted improvements in CAP conversion process parameters. These improvements result in MFSPs of \$3.49/GGE and \$3.73/GGE for the acids and BDO cases, respectively. The final 2030 example cases demonstrate a viable path to ultimately achieve the

BETO MFSP targets of \$2.5/GGE or lower, based solely on algal biomass, while capitalizing on the multi-fuel/product biorefinery concept of interest to BETO and avoiding small-market “niche” coproducts. That case assumes the same CAP processing targets as 2025 but with further reduced biomass costs tied to further improved cultivation performance. In these cases, analysis showed that diverting all TAGs to PU resulted in MFSPs below the target value of \$2.50/GGE (\$1.84/GGE and \$2.13/GGE for the acids and BDO cases, respectively). Accordingly, a portion of the TAG (9% for the acids case and 5% for the BDO case) was sent to fuels to demonstrate what would be required for future cases to meet targets of \$2.50/GGE.

As discussed above, we again note here that the PU co-production bars included in Figure 5 are intended to demonstrate proof-of-concept *examples* for the ability to valorize a portion of algal lipids for high-value PU production, based to date on a better-understood TEA modeling framework reflective of isocyanate-based foam PU processing (and associated market values). Given that such technology is reasonably well understood, being pursued commercially, and makes use of toxic isocyanates, NREL experimental work is not currently investigating such PU product routes. Instead, recent NREL work has focused on a more novel carbonation/diamine cross-linking route to yield NIPU with the potential to enable fully renewable chemistries. Good initial progress has been made under that route, and we defer to the associated experimental project reports for a full accounting of that work and resultant data [17, 18].

In summary, initial work found very rapid kinetics for NIPU synthesis when conducted on algal poly-unsaturated fatty acid (PUFA) substrates, with over 80% conversion of carbonated groups within the first 5 minutes and complete conversion in 30 minutes, given those substrates being highly reactive with many sites for epoxidation (resulting in solid/brittle end products, without measurable viscosities). However, the work identified ways to control the reaction rates through limiting the degree of carbonation, with PUFA substrates at low- to medium-carbonation degrees leading to NIPU products with measurable viscosities (varying significantly between 10–3,900 cP). Carbonated algal PUFA substrates also were seen leading to NIPU products ranging from very low to high tensile strength (1–570 Mpa Young’s modulus). NIPU polymer has been successfully prepared using both TAG and unsaturated FAMES as feedstocks; moreover, a cold-press fractionation method was developed to enrich unsaturated fatty acids, potentially allowing for the use of feedstocks with a low initial degree of unsaturation. In addition, multiple blowing methods for NIPU foam formation have been successfully tested, including the formation of a diamine-carbamate salt (forming CO₂ upon melting) and the use of citric acid with a bicarbonate salt (forming CO₂ upon reaction of the bicarbonate) (manuscript submitted). Still, given key gaps and uncertainties related to processing costs, manufacturing logistics, and product values for the NIPU route, NIPU coproduct is not currently reflected in the present SOT, but will be an important area for future work moving forward.

As discussed in other recent work [2, 25], we reiterate that the future projection scenarios shown in Figure 5 are by no means the *only* possible combinations of coproducts that support achieving less than \$2.5/GGE algal fuel goals, but are initial examples that demonstrate proof of concept based on recent activities to select these products for further TEA consideration. Likewise, NREL’s new CAP processing concept, although still under development, is also envisioned to enable an alternative path to meeting such out-year MFSP goals under a different process configuration, assuming current challenges with respect to MOT/catalytic upgrading can be

further optimized [2]. It also should be noted that CAP R&D is simultaneously investigating other alternate processing routes, including:

1. Fermentation to lactic acid (which could serve as a coproduct or an intermediate for fuel upgrading)
2. Fermentation to lipids (which could serve as an additional intermediate for both polyurethane and fuel)
3. Valorization of residual solids (with coproduct options including graphene, Algix or alternative polymer precursor, and animal/fish feed).

While the analysis of these options is less exhaustive than that of PU, they may still serve as alternate routes to achieving MFSP targets, especially for more challenging, high-protein feedstocks, which we intend to begin incorporating into future TEA focus.

Finally, Table 4 provides key technical and cost details associated with the various cases presented in Figure 5. This table shows that room for improvement exists moving forward beyond the current SOT baseline, particularly with respect to cultivation productivity (36% improvement), but also for key cost drivers in CAP conversion based on the current configuration, including pretreatment sugar yields (8% improvement) and sugar fermentation/upgrading yields (17% and 7% improvement in the acids [targeting butyric acid exclusively] and BDO pathways, respectively). Lipid extraction and upgrading yields have essentially achieved final target levels, but further room for improvement exists (i.e., around catalyst robustness and resistance to deactivation). Polyurethane conversion is based on complete conversion in epoxidation and ring opening, with foam production inputs consistent with mature technology, so it is also unlikely to contribute to further SOT improvements; however, advancements in the production of NIPUs could support a fully sustainable coproduct strategy, potentially at similar or decreased costs.

Note that the “conversion” contribution to MFSP for cases from 2020 onward in Table 4 reflects the net sum of all conversion process costs (“positive” bars in Figure 5) combined with the coproduct processing costs and revenues (“negative” bars in Figure 5); thus, the conversion MFSP values on the order of *negative* \$4/GGE or more for the future projection cases indicate that all non-feedstock conversion costs are outweighed by larger coproduct revenues, as required to compensate for high biomass costs inherent to microalgae farming. Finally, moving forward, other alternative CAP configurations may be further investigated as well, including the new CAP approach discussed previously or other variants that may support higher-protein algal biomass feedstocks.

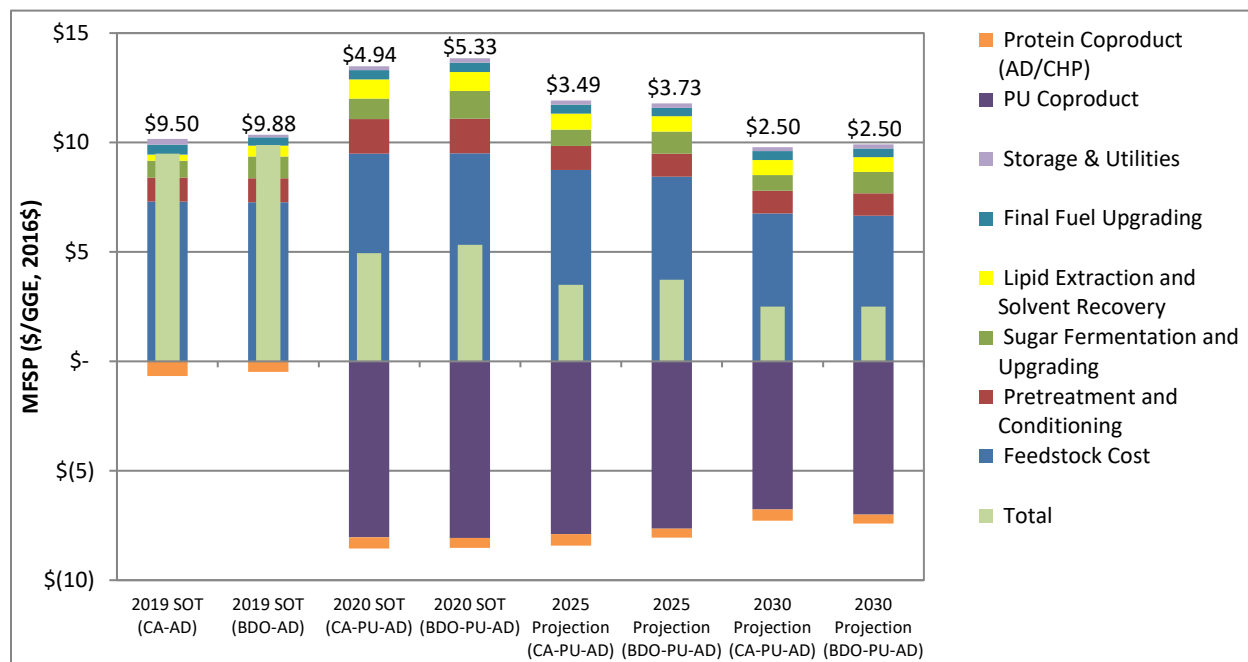


Figure 5: Summary of MFSP cost breakdowns for SOTs and future example projection scenarios (FA evaporation scenarios)

CA = sugar fermentation/upgrading to fuels via carboxylic acid intermediates; BDO = sugar fermentation/upgrading to fuels via 2,3-BDO intermediates; PU = polyurethanes derived from triglyceride fraction of lipids; all cases currently assume AD of protein residues, reflecting CAP configuration as depicted in Figure 1; 2030 cases are intentionally set to \$2.50/GGE by varying the ratio of triglycerides sent to fuel vs. PU

Table 4: Technical Overview Table for Cost and Process Metrics Associated with FY 2019–2020 SOT Cases, Compared to Example 2030 Projection Scenarios. SOT Cases Only Reflect FA Evaporation Scenarios for Simplicity.

Metric	2019 SOT (Acids) – FA Evap	2019 SOT (BDO) – FA Evap	2020 SOT (Acids-PU) – FA Evap	2020 SOT (BDO-PU) – FA Evap	2025 Projection (Acids-PU)	2025 Projection (BDO-PU)	2030 Projection (Acids-PU)	2030 Projection (BDO-PU)
MFSP (\$/GGE, 2016\$) ^a	\$9.50 [\$11.64]	\$9.88 [\$12.01]	\$4.94 [\$7.61]	\$5.33 [\$8.00]	\$3.49	\$3.73	\$2.50	\$2.50
Feedstock Contribution (\$/GGE, 2016\$) ^a	\$7.30 [\$9.44]	\$7.27 [\$9.40]	\$9.50 [\$12.16]	\$9.50 [\$12.17]	\$8.75	\$8.44	\$6.74	\$6.65
Conversion Contribution (\$/GGE, 2016\$) ^a	\$2.20 [\$2.20]	\$2.61 [\$2.61]	(\$4.54) [(\$4.54)]	(\$4.17) [(\$4.17)]	(\$5.25)	(\$4.70)	(\$4.24)	(\$4.15)
Yield (GGE/ton AFDW)	91.0	91.4	63.0	62.9	68.3	70.8	71.7	72.7
Renewable Diesel Blend-Stock Yield (GGE/ton AFDW)	53.7	64.2	45.3	40.8	48.9	45.0	51.5	46.6
Naphtha Yield (GGE/ton AFDW)	37.3	27.2	17.8	22.2	19.4	25.7	20.2	26.2
Finished Fuel Products Yield (GGE/acre/yr)	2,105	2,114	1,685	1,682	2,494	2,587	2,619	2,658
C Yield to Fuels from Biomass	46.3%	43.7%	31.1%	30.8%	32.8%	33.8%	34.5%	34.7%
C Yield to Coproducts from Biomass (algal carbon only)	N/A	N/A	20.6%	20.6%	20.5%	20.5%	18.6%	19.4%
Feedstock								
Feedstock Cost (\$/ton AFDW) ^a	\$670 [\$866] ^b	\$670 [\$866] ^b	\$603 [\$772] ^b	\$603 [\$772] ^b	\$602	\$602	\$488	\$488
Year-Average Cultivation Productivity (g/m ² /day AFDW)	15.9	15.9	18.4	18.4	20	20	25	25
Max Seasonal Variability (max:min productivity)	4.2:1	4.2:1	3.8:1	3.8:1	3.0:1	3.0:1	3.0:1	3.0:1
Harvested Biomass Lipid Content (dry wt% as FAME)	26% ^b	26% ^b	26% ^b	26% ^b	26%	26%	26%	26%
Harvested Biomass Concentration (g/L AFDW)	0.49	0.49	0.46	0.46	0.5	0.5	0.5	0.5
Pretreatment + Conditioning								
Solids Loading (wt%)	20% ^c	20% ^c	20% ^c	20% ^c	20%	20%	20%	20%
Acid Loading (wt% versus feed water rate)	2%	2%	2%	2%	1%	1%	1%	1%
Fermentable Sugar Release (“glucose yield”)	74%	74%	83%	83%	90%	90%	90%	90%
Glucan to Degradation Products	1.5%	1.5%	1.5%	1.5%	0.3%	0.3%	0.3%	0.3%
Hydrolysate Solid-Liquid Separation	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Metric	2019 SOT (Acids) – FA Evap	2019 SOT (BDO) – FA Evap	2020 SOT (Acids-PU) – FA Evap	2020 SOT (BDO-PU) – FA Evap	2025 Projection (Acids-PU)	2025 Projection (BDO-PU)	2030 Projection (Acids-PU)	2030 Projection (BDO-PU)
Sugar Fermentation + Catalytic Upgrading								
Fermentation Productivity (g/L-hr)	0.3	1.3 (56-h batch time)	0.3	1.3 (56-h batch time)	2.0	2.0 (36-h batch time)	2.0	2.0 (36-h batch time)
Product titer (g/L)	N/A ^d	73	N/A ^d	73	N/A ^d	90	N/A ^d	90
Glucose to Product ^e	92%	74%	92%	74%	95%	95%	95%	95%
Mannose to Product ^e	92%	55%	92%	55%	95%	95%	95%	95%
Glycerol to Product ^e	92%	0%	92%	0%	95%	95%	95%	95%
Overall Fermentation Yield to Product (g/g total sugars) ^e	0.48	0.34	0.48	0.34	0.50	0.48	0.50	0.48
Catalytic Upgrading Carbon Yield to HDO Feed ^f	57%	56%	83%	98%	83%	98%	83%	98%
Lipid Processing								
Solvent Loading (nonpolar:EtOH:dry biomass ratio, wt)	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1	2.7:1.1:1
Total Convertible Lipid Extraction Yield	96%	96%	96%	96%	96%	96%	96%	96%
Lipid Impurity Partition to Extract	<11.5%	<11.5%	<11.5%	<11.5%	<11.5%	<11.5%	<11.5%	<11.5%
Fuel Finishing Renewable Diesel Blend-Stock Yield (wt% of total feed) ^g	51.9%	60.6%	64.4%	56.6%	64.5%	55.8%	64.3%	56.0%
Fuel Finishing Naphtha Yield (wt% of total feed) ^g	35.9%	25.3%	25.3%	30.5%	25.6%	31.6%	25.3%	31.2%
Fuel Finishing H ₂ Consumption (wt% of total feed) ^g	3.2%	3.0%	2.6%	2.2%	2.6%	2.2%	2.6%	2.2%
Polyol/Polyurethane Production								
Polyurethane yield from TAG (w/w TAG) ^h	N/A	N/A	1.60	1.60	1.60	1.60	1.60	1.60
% TAG Diversion to Polyurethane Coproduct (%)	N/A	N/A	100%	100%	100%	100%	91%	95%
Overall Polyurethane Yield from Algae (wt% AFDW)	N/A	N/A	22.4%	22.4%	22.4%	22.4%	20.8%	21.6%
Protein/Stillage Processing								
N/P Recycle to Ponds (% of biomass feed to CAP)	100%/76%	100%/46%	100%/73%	100%/51%	100%/73%	100%/54%	100%/73%	100%/53%
AD Biogas Yield (L CH ₄ /g TS)	0.26	0.25	0.23	0.22	0.26	0.25	0.26	0.25

^a First values represent unlined pond base case; values in brackets represent fully lined pond scenario

^b SOT based on ASU production of *Desmodesmus*, *Scenedesmus*, *Monoraphidium*, and/or *Picochlorum* (as applicable) overlaid with target HCSD composition

^c Experimental work conducted at pretreatment solids content varying around 20%, expected to perform the same as 20%

^d Acids fermentation case based on continuous *in situ* acid removal across pertractive membrane

^e "Product" refers to acetic/butyric acids for the acids case and 2,3-BDO for the BDO case

^f Represents overall catalytic upgrading yield of fermentation intermediates (after recovery) through feed to final fuel finishing (hydrotreating) step

^g Final "fuel finishing" step is a combined hydrotreater to upgrade lipids plus the final intermediate from the sugar conversion train

^h Only includes TAG utilized for PU production.

Sustainability Metric Indicators

In addition to the TEA results noted above, here we also report on associated sustainability “indicators” attributed to the algae CAP SOT model. In keeping with recent BETO guidance for all formal life cycle assessment sustainability metrics to be handled by Argonne National Laboratory 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 life cycle assessment parameters such as greenhouse gas emissions or fossil energy consumption in this report (but are currently working to provide the input/output inventories to partners at Argonne National Laboratory). Instead, Table 5 summarizes key sustainability indicators as may be taken directly from the Aspen Plus process. Namely, for the CAP conversion SOT, this includes mass and carbon yield to fuels, carbon yield to coproducts, facility power and natural gas demands, and freshwater demands for the conversion process. While most of the parameters are fairly comparable between the two pathways, the BDO pathway requires more heat and thus a higher natural gas import, which is co-fired in the AD biogas turbine, but which in turn also leads to more power generation through the turbine that translates to a larger net power export versus the BDO pathway. The process input/output inventories furnished to Argonne National Laboratory for subsequent life cycle assessment supply chain sustainability analysis (SCSA) are summarized in Appendix B.

Table 5. Sustainability Indicators for FY 2020 SOT CAP Models

Parameter		FY 2020 SOT Fermentation Pathway	
		Acids	BDO
Fuel Yield by Weight of Biomass	GGE per dry ton biomass	63.0	62.9
Carbon Efficiency to Fuels	% of algal C used	31.1	30.8
Carbon Efficiency to Coproduct	% of algal C used	20.6	20.6
Electricity Import/Export	kWh/GGE	-5.04 (export)	-6.01 (export)
Natural Gas Import	MJ/GGE	104	173
Water Consumption ^a	m ³ /day	1,480	2,380
Water Consumption ^a	gal/GGE	15.3	24.6

^a Reflects freshwater makeup for the CAP process, independent of water recycle to cultivation facility

Concluding Remarks

The updated CAP configuration and process parameters, combined with updated FY 2020 SOT biomass costs (MBSPs) and associated yields from the front-end algae farm model, translate to an **estimated FY 2020 SOT minimum fuel selling price of \$6.12/GGE (acids pathway) or \$6.50/GGE (BDO pathway) for the ASU evaporation MBSP basis, or \$4.94/GGE and \$5.33/GGE (acids versus BDO) for the FA evaporation basis (all results in 2016\$)** for the unlined pond base case. SOT fuel costs for the alternative fully lined pond scenario would increase to \$8.80/GGE or \$9.80/GGE for the acids and BDO cases, respectively, under baseline ASU evaporation rates.

The net benefit of all the improvements considered in the FY 2020 SOT is substantial, resulting in a 40%–48% decrease in MFSP compared to FY 2019 SOT results. This difference can be largely attributed to new inclusion of the polyurethane coproduct, which is responsible for roughly 75% of the change in MFSP. Updated MBSPs from the upstream cultivation process also account for a substantial (19%) amount of the change, with the remainder attributed to improvements in dilute acid pretreatment and seasonal storage. Between the two sugar fermentation pathways for intermediate fuel precursor production, the acids pathway continues to indicate slightly lower MFSPs in the present SOT (roughly \$0.38/GGE lower for acids than BDO), primarily due to better fermentation performance/yields toward acids, the preliminary and unoptimized nature of the *Zymomonas* BDO strain engineered for mannose utilization, and lower acids upgrading costs. Moving forward, this difference would likely shrink as BDO fermentation were to improve or conditions were further optimized for higher titers.

Beyond current SOT benchmarks, to increase yields and reduce MFSP cost on the conversion side moving forward under this CAP configuration reflected here, further room exists to optimize pretreatment conditions and improve fermentable sugar yields (i.e., carbohydrate hydrolysis to monomeric sugars and fermentation yield to butyric acid or BDO), which may be achieved in one instance by potentially reducing acid loading and targeting increased sugar oligomers followed by a low-cost oligomer “hold” step to convert oligomers to fermentable monomers. Additionally, while lipid extraction and upgrading yields have been demonstrated near their final goals for this CAP approach, further room for improvement exists around improving catalyst stability and activity for HDO plus HI functionalities in the presence of algal lipid impurities, and on better understanding ramifications on hydrotreater design for co-processing both lipids and the final intermediate compounds from sugar train upgrading through the same fuel finishing reactor.

Polyurethane production costs are unlikely to change significantly due to the relatively mature technology level; however, further advancements in NIPU research may warrant inclusion in future SOTs. First, a better understanding of key processing design/cost considerations would be required, as well as product applications and price values for such a material. It is possible that NIPU could be produced at a similar cost as conventional PU (given the similarities between each process), with more preferable implications on safety, environmental, and sustainability aspects. These benefits may even justify a higher selling price for NIPUs, which would further close the gap between SOT cost estimations and future targets.

Future experimental plans also intend to continue investigating alternative CAP processing schemes for different algal biomass compositions, including more optimal uses of algal protein.

In 2019, such alternative processing strategies began to be pursued experimentally, starting first with nutrient deplete (high-carbohydrate/high-lipid) biomass, and demonstrating preliminary proof of concept for key new unit operations exhibiting an ability to co-convert both carbohydrates and protein into fuel precursors. Experimental work so far in this area has demonstrated reasonable yields for solubilized proteins and carbohydrates, but has shown challenges associated with conversion of solids. Moving forward, a number of options will be pursued to better understand and optimize those processing steps, and additionally to consider modifications to the process to accommodate and better valorize high-protein biomass. Those efforts would provide important “risk mitigation” strategies for the CAP pathway in the event that the targeted HCSD-type compositions could not be achieved as projected and instead cultivation trials continued to produce higher-protein/lower-lipid biomass for the foreseeable future. In all cases involving high-protein biomass, inclusion of one or more value-added coproducts with sufficiently large market volumes will continue to be a central element for achieving BETO goals of \$2.5/GGE algal biofuels while supporting commodity-scale deployment of such algal biorefinery concepts.

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Appendix A. TEA Summary Sheet for Base Case CAP SOT Benchmark Model

Acids Case (FA Evaporation MBSP Scenario, 2016\$)

Combined Algal Processing to Fuels and Bioproducts Process Engineering Analysis

Cost Year Basis:		2016 \$
MFSP (Gasoline Equivalent Basis):		\$4.94 /GGE
Contributions:	Feedstock	\$9.49 /GGE
	Conversion	-\$4.54 /GGE

Total Fuel Production (RDB + Naphtha + Ethanol):		8.43 MMGGE/yr
	RDB Production:	6.05 MMGGE/yr
	Naphtha Production:	2.37 MMGGE/yr
	Ethanol Production:	0.00 MMGGE/yr
Total Fuel Yield (RDB + Naphtha + Ethanol):		63.02 GGE / dry U.S. ton feedstock
	Feedstock Cost:	\$603 dry U.S. Ton algal biomass (ash free)
	Internal Rate of Return:	10%
	Equity Percent of total Investment:	40%

Capital Costs		Manufacturing Costs (cents/GGE)	
A100: Pretreatment and Conditioning	\$25,100,000	Feedstock	948.7
A200: Carboxylic Acid Fermentation and Distillation	\$14,400,000	Pretreatment Chemicals	49.5
A200: 2,3-BDO Fermentation and Upgrading	\$0	A200 chemicals	27.8
A300: Lipid Extraction and Separation	\$16,700,000	Lipid Extraction and Cleanup Chemicals	21.7
A400: Product Purification and Upgrading	\$4,600,000	Hydrogen	15.2
A500: Protein/Residual Processing	\$4,700,000	Polyurethane Inputs	350.0
A600: Combined Heat and Power	\$6,400,000	Supplemental Natural Gas	45.8
A700: Utilities & Storage	\$3,100,000	Remaining Raw Materials	2.0
Total Installed Equipment Cost	\$75,000,000	Coproduct Credits	-1422.1
		Other Credits (recycled nutrients, etc.)	-88.7
Added Direct + Indirect Costs	\$209,300,000	Exported Electricity	-28.8
(% of TCI)	73.62%	Catalysts	3.7
		Fixed Costs	134.1
Total Capital Investment (TCI)	\$284,300,000	Capital Depreciation	134.1
		Average Income Tax	32.7
Installed Equipment Cost/Annual GGE	\$8.90	Average Return on Investment	268.7
Total Capital Investment/Annual GGE	\$33.74		
		Manufacturing Costs (\$/yr)	
Loan Rate	8%	Feedstock	\$79,900,000
Term(years)	10	Pretreatment Chemicals	\$4,200,000
Capital Charge Factor (Computed)	0.089	A200 chemicals	\$2,300,000
		Lipid Extraction and Cleanup Chemicals	\$1,800,000
Carbon Retention Efficiencies:		Hydrogen	\$1,300,000
Total Carbon Efficiency to Fuel and Products	59.3%	Polyurethane Inputs	\$29,500,000
(Fuel C/Biomass C)		Supplemental Natural Gas	\$3,900,000
RDB (RDB C/Biomass C)	22.4%	Remaining Raw Materials	\$200,000
Naphtha (Naphtha C/Biomass C)	8.7%	Coproduct Credits	-\$119,800,000
Polyurethane (total C in PU/Biomass C)	28.2%	Other Credits (recycled nutrients, etc.)	-\$7,500,000
Polyurethane (algal C in PU/Biomass C)	20.6%	Exported Electricity	-\$2,400,000
		Catalysts	\$300,000
		Fixed Costs	\$11,300,000
		Capital Depreciation	\$11,300,000
		Average Income Tax	\$2,800,000
		Average Return on Investment	\$22,600,000
Fuel Yields			
RDB Production (U.S. ton/yr)	18,627		
Naphtha Production (U.S. ton/yr)	7,309		

BDO Case (FA Evaporation MBSP Scenario, 2016\$)

Combined Algal Processing to Fuels and Bioproducts Process Engineering Analysis

Cost Year Basis:	2016 \$
MFSP (Gasoline Equivalent Basis):	\$5.33 /GGE
Contributions:	
Feedstock	\$9.50 /GGE
Conversion	-\$4.17 /GGE
Total Fuel Production (RDB + Naphtha + Ethanol):	8.41 MMGGE/yr
RDB Production:	5.45 MMGGE/yr
Naphtha Production:	2.96 MMGGE/yr
Ethanol Production:	0.00 MMGGE/yr
Total Fuel Yield (RDB + Naphtha + Ethanol:	62.92 GGE / dry U.S. ton feedstock
Feedstock Cost:	\$603 dry U.S. Ton algal biomass (ash free)
Internal Rate of Return:	10%
Equity Percent of total Investment:	40%

Capital Costs		Manufacturing Costs (cents/GGE)	
A100: Pretreatment and Conditioning	\$25,100,000	Feedstock	950.2
A200: Carboxylic Acid Fermentation and Distillation	\$0	Pretreatment Chemicals	49.6
A200: 2,3-BDO Fermentation and Upgrading	\$19,900,000	A200 chemicals	27.6
A300: Lipid Extraction and Separation	\$16,700,000	Lipid Extraction and Cleanup Chemicals	21.7
A400: Product Purification and Upgrading	\$4,700,000	Hydrogen	13.7
A500: Protein/Residual Processing	\$4,000,000	Polyurethane Inputs	350.6
A600: Combined Heat and Power	\$8,200,000	Supplemental Natural Gas	76.3
A700: Utilities & Storage	\$3,300,000	Remaining Raw Materials	3.2
Total Installed Equipment Cost	\$81,900,000	Coproduct Credits	-1424.4
Added Direct + Indirect Costs	\$215,600,000	Other Credits (recycled nutrients, etc.)	-100.6
(% of TCI)	72.47%	Exported Electricity	-34.4
Total Capital Investment (TCI)	\$297,500,000	Catalysts	5.5
Installed Equipment Cost/Annual GGE	\$9.74	Fixed Costs	137.3
Total Capital Investment/Annual GGE	\$35.37	Capital Depreciation	137.9
		Average Income Tax	34.4
		Average Return on Investment	284.4
		Manufacturing Costs (\$/yr)	
Loan Rate	8%	Feedstock	\$79,900,000
Term(years)	10	Pretreatment Chemicals	\$4,200,000
Capital Charge Factor (Computed)	0.088	A200 chemicals	\$2,300,000
Carbon Retention Efficiencies:		Lipid Extraction and Cleanup Chemicals	\$1,800,000
Total Carbon Efficiency to Fuel and Products	59.0%	Hydrogen	\$1,100,000
(Fuel C/Biomass C)		Polyurethane Inputs	\$29,500,000
RDB (RDB C/Biomass C)	20.1%	Supplemental Natural Gas	\$6,400,000
Naphtha (Naphtha C/Biomass C)	10.7%	Remaining Raw Materials	\$300,000
Polyurethane (total C in PU/Biomass C)	28.2%	Coproduct Credits	-\$119,800,000
Polyurethane (algal C in PU/Biomass C)	20.6%	Other Credits (recycled nutrients, etc.)	-\$8,500,000
		Exported Electricity	-\$2,900,000
		Catalysts	\$500,000
		Fixed Costs	\$11,600,000
		Capital Depreciation	\$11,600,000
		Average Income Tax	\$2,900,000
		Average Return on Investment	\$23,900,000
Fuel Yields			
RDB Production (U.S. ton/yr)	16,776		
Naphtha Production (U.S. ton/yr)	9,033		

Appendix B. Life Cycle Inventory for 2020 CAP SOT Models

Acids Case: SOT input and output inventory data for the modeled CAP process. (Note: hourly rates are based on annual averages over all modeled seasons.)

Resource Consumption	kg/hr
Feedstock (AFDW basis)	15,312
<i>Pretreatment</i>	
Sulfuric Acid (93% pure)	1,365
Ammonia	441
<i>Lipid Extraction and Cleanup</i>	
Hexane Requirement	80
Ethanol	32
Phosphoric acid (oil cleanup)	44
Silica (oil cleanup)	4
Clay (oil cleanup)	9
<i>Carboxylic Acid Conversion</i>	
Corn Steep Liquor	694
Diammonium Phosphate	72
Hydrotalcite	1
Flocculant	61
Hexane	1
Ketonization Catalyst (ZrO ₂)	0.03
Condensation Catalyst (Niobic Acid)	0.21
<i>Final Fuel Upgrading (HDO/HI)</i>	
Hydrogen	100
One-Step HDO/HI Catalyst (1% Pt/SAPO-11)	0.22
<i>Polyurethane Production</i>	
Formic Acid	331
H ₂ O ₂	525
Catalysts and Other Chemicals	2,496
Nitrogen	50
Toluene Diisocyanate	911
Diethanolamine	9
Surfactant	17
<i>Other Resource Consumption</i>	
Supplemental Natural Gas	1,984
Process Water	61,777
Output Streams	
AD Digestate Cake (dry basis total flow)	3,541
AD Digestate Cake Bioavailable N	18
AD Effluent NH ₃	222
AD Effluent DAP	105
Recycle Water (excluding N/P nutrients)	99,883
<i>Direct Air Emissions</i>	
H ₂ O	32,820
<i>CO₂ Recycle</i>	
CO ₂ (Biogenic)	8,775
CO ₂ (Fossil)	5,981
Biomass Loss from Storage	
Algae Biomass Loss from Wet Storage	321

BDO Case: SOT input and output inventory data for the modeled CAP process. (Note: hourly rates shown based on annual averages over all modeled seasons.)

Resource Consumption	kg/hr
Feedstock (AFDW basis)	15,312
<i>Pretreatment</i>	
Sulfuric Acid (93% pure)	1,365
Ammonia	441
<i>Lipid Extraction and Cleanup</i>	
Hexane Requirement	80
Ethanol	32
Phosphoric Acid (oil cleanup)	44
Silica (oil cleanup)	4
Clay (oil cleanup)	9
<i>2,3-BDO Conversion</i>	
Corn Steep Liquor	103
DAP	13
Hydrogen	78
Flocculant	61
Dehydration Catalyst	0.06
Oligomerization Catalyst	0.12
<i>Final Fuel Upgrading (HDO/HI)</i>	
Hydrogen	90
One-Step HDO/HI Catalyst (1% Pt/SAPO-11)	0.23
<i>Polyurethane Production</i>	
Formic Acid	331
H ₂ O ₂	525
Catalysts and Other Chemicals	2,496
Nitrogen	50
Toluene Diisocyanate	911
Diethanolamine	9
Surfactant	17
<i>Other Resource Consumption</i>	
Supplemental Natural Gas	3,301
Process Water	98,968
Output Streams	
AD Digestate Cake (dry basis total flow)	3,374
AD Digestate Cake Bioavailable N	17
AD Effluent NH ₃	216
AD Effluent DAP	74
Recycle Water (excluding N/P nutrients)	102,324
<i>Direct Air Emissions</i>	
H ₂ O	38,613
<i>CO₂ Recycle</i>	
CO ₂ (Biogenic)	8,647
CO ₂ (Fossil)	9,594
Biomass Loss from Storage	
Algae Biomass Loss from Wet Storage	321