ANL/ESD-22/5 Rev. 1

Supply Chain Sustainability Analysis of Renewable Hydrocarbon Fuels via Indirect Liquefaction, Hydrothermal Liquefaction, Combined Algal Processing, and Biochemical Conversion: Update of the 2021 State-of-Technology Cases

Energy Systems Division

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by
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1 INTRODUCTION

The Department of Energy's (DOE) Bioenergy Technologies Office (BETO) aims to develop and deploy technologies to transform renewable biomass resources into commercially viable, high-performance biofuels, bioproducts, and biopower through public and private partnerships. BETO and its national laboratory teams conduct in-depth techno-economic assessments (TEA) of biomass feedstock supply and logistics and conversion technologies to produce biofuels. There are two general types of TEAs: A *design case* outlines a target case (future projection) for a particular biofuel pathway. It informs R&D priorities by identifying areas in need of improvement, tracks sustainability impact of R&D, and provides goals and benchmarks against which technology progress is assessed. A *state of technology* (SOT) analysis assesses progress within and across relevant technology areas based on actual results at current experimental scales relative to technical targets and cost goals from design cases, and includes technical, economic, and environmental criteria as available.

In addition to developing a TEA for a pathway of interest, BETO also performs a supply chain sustainability analysis (SCSA). The SCSA takes the life-cycle analysis approach that BETO has been supporting for about 20 years. It enables BETO to identify energy consumption, environmental, and sustainability issues that may be associated with biofuel production. Approaches to mitigating these issues can then be developed. Additionally, the SCSA allows for comparison of energy and environmental impacts across biofuel pathways in BETO's research and development portfolio.

This technical report describes the SCSAs for the production of renewable hydrocarbon transportation fuels via a range of conversion technologies in the 2021 SOTs: (1) renewable high octane gasoline (HOG) via indirect liquefaction (IDL) of woody lignocellulosic biomass to syngas (note that the IDL pathway in this SCSA represents the bench-scale experiments in 2021, with corresponding conceptual scale-up assumptions (Harris et al. 2022); (2) renewable diesel (RD) via hydrothermal liquefaction (HTL) of wet sludge from a wastewater treatment plant; (Snowden-Swan et al. 2022) (3) renewable hydrocarbon fuels via biochemical conversion of herbaceous lignocellulosic biomass (Davis et al. 2022; Lin et al. 2020); (4) RD via HTL of algae produced as part of wastewater remediation services in a municipal water resource recovery facility (WRRF) (Zhu et al. 2022); and (5) renewable hydrocarbon fuels via combined algae processing (CAP) (Wiatrowski et al. 2022). Table 1 summarizes the feedstock options, conversion technologies, and finished products of the five 2021 SOT pathways. For simplicity and comparison with petroleum diesel, all LCI and LCA metrics for the biochemical conversion, HTL, and CAP pathways are reported on an RD basis, using an energy-based allocation method that allocates the sustainability impacts of both naphtha- and diesel-range hydrocarbon fuel products based on their energy contents.

Table 1 2021 SOT pathways for SCSAs

Pathway	Feedstock	Conversion	Finished Products
HOG via IDL	50% clean pine and 50% logging residues	IDL	HOG
RD via HTL	Wastewater treatment plant sludge	HTL	RD and naphtha
Renewable hydrocarbon fuels via biochemical conversion	Corn stover	Biochemical conversion	RD and naphtha
RD via HTL	Wastewater algae	HTL	RD and naphtha
Renewable hydrocarbon fuels via CAP	Algae	CAP	RD and naphtha

This report focuses on the environmental performance of these biofuel production pathways in their 2021 SOT cases. The results of these renewable hydrocarbon fuel pathways in these SCSA analyses update those for the respective 2020 SOT case (Cai et al. 2021). They also provide an opportunity to examine the impact of technology improvements in both biomass feedstock production and biofuel production that have been achieved in 2021 SOTs on the sustainability performance of these renewable transportation fuels. The SCSA results also reflect updates to Argonne National Laboratory's Greenhouse gases, Regulated Emissions, and Energy use in Technologies (GREET®) model, which was released in October 2021 (Wang et al. 2021). These GREET updates include the production of natural gas, electricity, and petroleum-based fuels that can influence biofuels' supply chain greenhouse gas (GHG) (CO_2, CH_4, and N_2O) emissions, water consumption, and air pollutant emissions. GHG emissions, water consumption, and nitrogen oxides (NO_x) emissions are the main sustainability metrics assessed in this analysis. In this analysis, we define water consumption as the amount of water withdrawn from a freshwater source that is not returned (or returnable) to a freshwater source at the same level of quality. Life-cycle fossil energy consumption and net energy balance, which is the life-cycle fossil energy consumption deducted from the renewable biofuel energy produced, are also assessed.

Figure 1 shows the stages in the supply chain that are considered and the data sources used in the SCSA of HOG via IDL, and renewable hydrocarbon fuels from biochemical, algae HTL, algae CAP, and sludge HTL conversion. In this analysis, we consider the upstream impacts of producing each energy and chemical input to the supply chain.

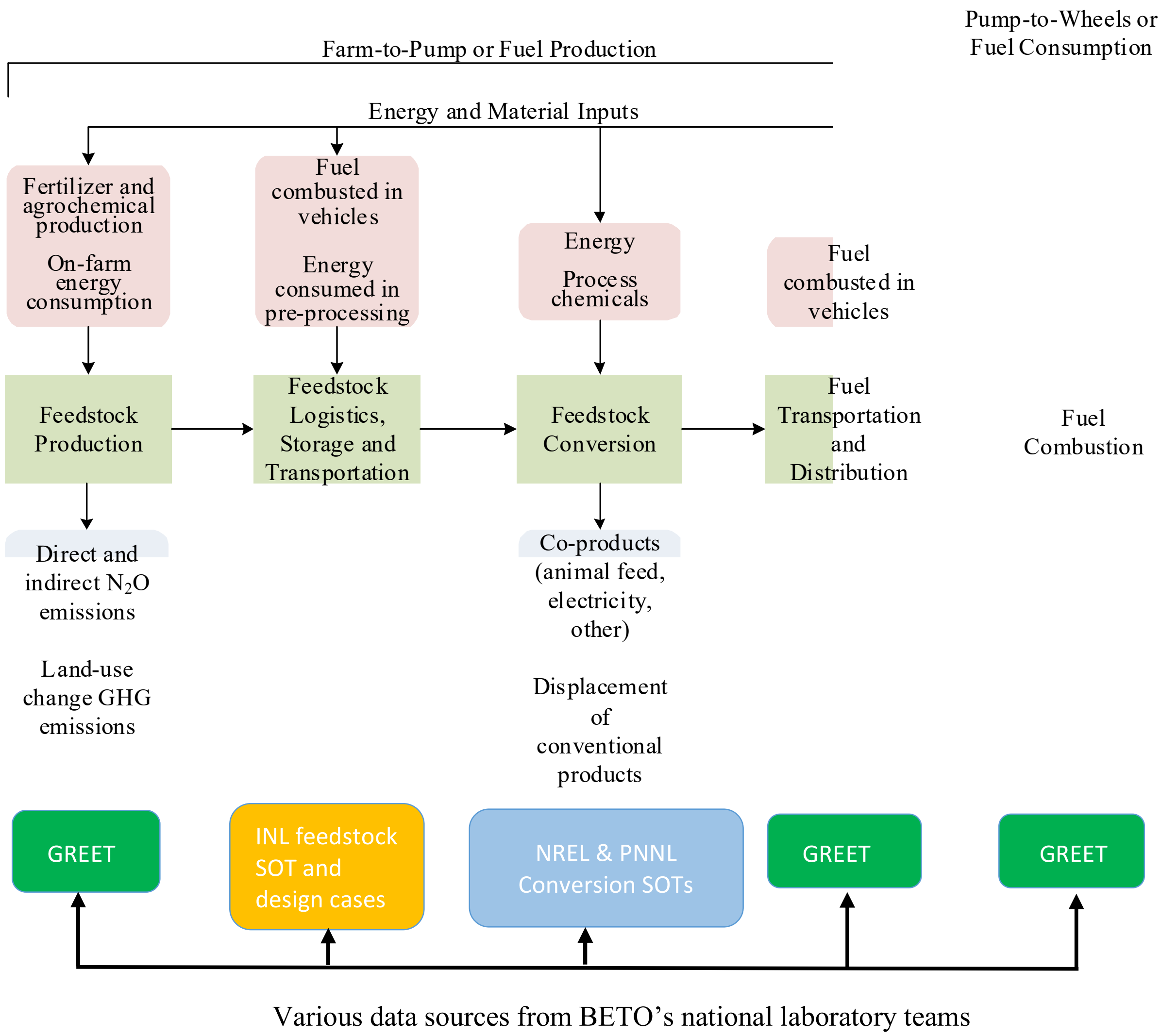


Figure 1 General Stages Considered and Data Sources Used in the Supply Chain Sustainability Analyses for HOG via IDL and Renewable Hydrocarbon Fuels from Biochemical Conversion

2 METHODS AND DATA

Argonne National Laboratory's GREET model was used to generate the SCSA results for the 2021 SOT cases of the five biofuel pathways. The GREET model, developed with the support of DOE, is a publicly available tool for the life-cycle analysis of transportation fuels, and permits users to investigate the energy and environmental impacts of numerous fuel types and vehicle technologies. GREET computes fossil, petroleum, and total energy use (including renewable energy in biomass), GHG emissions, water consumption, and emissions of six air pollutants: carbon monoxide (CO), volatile organic compounds (VOCs), NO_x, sulfur oxides (SO_x), and particulate matter with an aerodynamic diameter below 10 micrometers (PM_{10}) and below 2.5 micrometers ($PM_{2.5}$), in the various fuel production pathways. Regular updates and expansion of the GREET model enable timely characterization of recent technology development and any modifications and improvement in the supply chain operations of energy and chemical products that are required for the biofuel production analyzed in this report.

For biofuel pathways with a significant amount of co-products, e.g., the biochemical conversion pathway, we will apply different co-product handling methods including the biorefinery-level method as described in Cai et al. (2021) to address the co-product effects.

As discussed by Cai et al. (2018), each co-product method has its strengths and limitations. We present the SCSA results with all these methods and discuss their implications to illuminate and inform stakeholders of the significant sustainability effects of co-products in such biorefinery designs.

2.2 Material and Energy Requirement of Feedstock Production and Logistics

2.2.1 Herbaceous and Woody Biomass Production and Logistics

For the herbaceous feedstock, the 2021 SOT used air classification to clean up the 3-pass corn stover down to a 6% ash content. Meanwhile, the switch to only 3-pass corn stover lowered the energy requirement of harvest compared to a 2-pass harvest practice. For the woody feedstock, the feedstock production, logistics, and the blending strategies considered in the 2020 SOT remain the same and are applied to conduct the SCSA of the 2021 SOT of the IDL pathways.

The National Renewable Energy Laboratory (NREL) modeled an algal feedstock (Klein and Davis 2022) used for the algae CAP pathway. Pacific Northwest National Laboratory (PNNL) modeled wet sludge from wastewater treatment plants as feedstock for the sludge HTL pathway (Snowden-Swan et al. 2022).

Wet sludge for the HTL pathway is from a wastewater treatment plant (WWTP) that is co-located with an HTL plant. The wet sludge has a moisture content of 75%-80% and a dry matter content of about 15% that primarily consists of carbon, oxygen, and ash, with a small amount of hydrogen, nitrogen, phosphorus, and sulfur (Snowden-Swan et al. 2022).

2.2.2 Algae Biomass Cultivation

Algae cultivation for CAP conversion is modeled from the algae farm design report (Davis and Klein 2022; Davis et al. 2016), which assumes sourcing of CO_2 through the capture of flue gas from coal-fired power plants. Energy requirements for algae cultivation assume a 5,000-cultivation-acre farm facility, a size selected based on optimal economy of scale considerations. All cultivation and conversion cases considered in this SCSA are based on the production of saline algae species in Florida (based on associated local seasonal evaporation rates) for consistency with prior SOT cases. This is overlaid with algal biomass productivity data that has reflected experimental cultivation trials at the ASU AzCATI test-bed site since the 2017 SOT.

In the 2021 SOT case (Davis and Klein 2022), high purity CO_2 produced from carbon capture of flue gas from coal-fired power plants and other point sources is transported to the farm gate via a high-pressure pipeline. An energy demand of 0.63 mega-joules (MJ) per kilogram of CO_2 is assumed for CO_2 capture and pipeline delivery (attributed to advanced second-generation carbon capture technologies). The process assumes a continuous mode of cultivation and harvesting to maximize the on-stream utilization of all capital costs. Once harvested, the biomass is routed through three stages of dewatering to reach a final solids content of 20 wt% (ash-free dry weight, AFDW). The harvested biomass composition was set to a future target projection consistent with compositional attributes previously measured for mid-harvest, high-carbohydrate *Scenedesmus* (Davis and Klein, 2022). Figure 2 shows a general block-flow diagram of the process. Further details of the process design are given in the report (Davis and Klein 2022). In these SCSAs, saline scenarios with minimally lined ponds are considered for the downstream conversion of algal biomass to fuels and co-products.

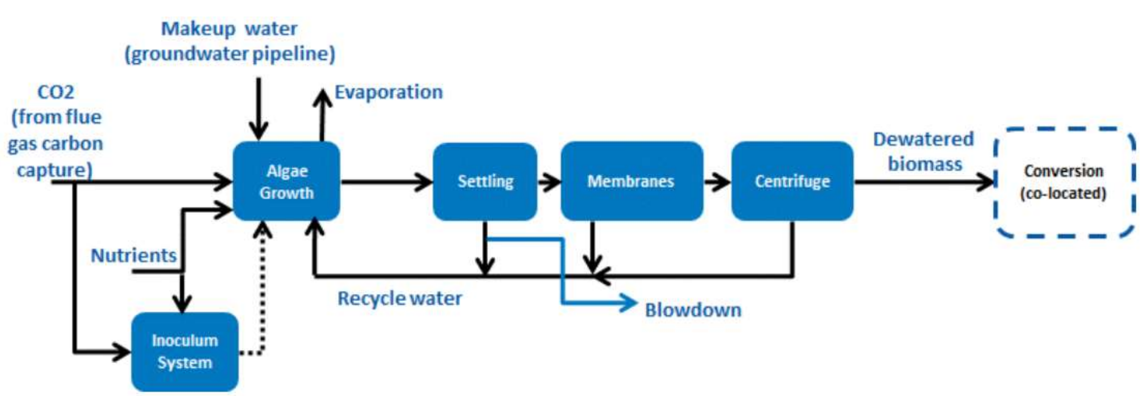


Figure 2 Process Flow Diagram of the Open Pond Algae Farm Model

Table 2 summarizes material and energy inputs and outputs of the 2021 algae farm model SOT. The input nutrient demands represent the gross requirements for cultivation, prior to accounting for any recycles from downstream conversion (these are credited in the respective algal conversion models instead).

Table 2 Algal Biomass Production and Resource Requirement (Annual Averages, Hourly Net Rates Inclusive of Downstream Recycles Reflect Average Daily Rates Divided by a 24-Hour Day)

	2021 SOT
	Algae for CAP
Products, kg/hr	
Algal biomass (AFDW)	14,675
Algal biomass (total including ash)	15,038
Make-up resource requirement, kg/hr	
CO_2	32,656
Ammonia	294
Diammonium phosphate	142
Total process water input (saline water)	511,367
Electricity demand, kW	8,850
Algae lost in blowdown	2

Prior SOTs for the algae HTL pathway were based on experimental testing and analysis of farmed microalgae consistent with NREL's farm model. This year, PNNL's R&D pivoted to investigation of low/no-cost algae resources to address an increasing interest in reducing feedstock costs for more near-term opportunities. As a result, the feedstock chosen for the 2021 SOT is algae that is grown as part of wastewater treatment services at a WRRF. As such, the feedstock is assumed to be a by-product of the WRRF's water remediation environmental service. Informed by the industry partner's experience (Zhu et al. 2022), nutrient burdens associated with algae growth are assumed to be supplied by the wastewater components. In addition, power needs associated with algae growth are fully attributed to the WRRF operations and not the algae feedstock. More details are provided in Section 2.3.5 and Zhu et al. (2022).

2.3 Material, Energy, and Water Requirements of Conversion Processes

2.3.1 Indirect Liquefaction (IDL)

The 2021 SOT case for the IDL pathway features a processing capacity of 2,205 U.S. short tons of dry feedstock per day at the biorefinery. The high-octane-gasoline (HOG) yield at the biorefinery is 55.6 gallons, or 6.0 MMBtu per dry U.S. short ton of feedstock, which is an increase of 1% relative to the 2020 SOT case (Harris et al. 2021). Figure 3 shows a simplified process flow diagram (PFD) of the IDL pathway. The process includes indirect steam gasification of a woody biomass, followed by gas conditioning and cleanup via steam reforming, scrubbing, and acid gas removal. The clean syngas is converted to methanol and then DME in two steps; the DME is then converted to HOG. The current research efforts focus on the DME-to-HOG step in which DME undergoes homologation to form primarily branched paraffin hydrocarbons. For details regarding the conversion process, see the detailed design report (Tan et al. 2015).

Table 3 lists the direct material, energy, and water consumption for the modeled IDL conversion process at the plant in the 2021 SOT case (Harris et al. 2021). Boiler feed water chemicals and cooling tower chemicals are not considered in the analysis due to a lack of information on their makeup. The impact of excluding such chemicals would likely be small, given their very low consumption levels (a combined 3.4 g/MMBTU of HOG).

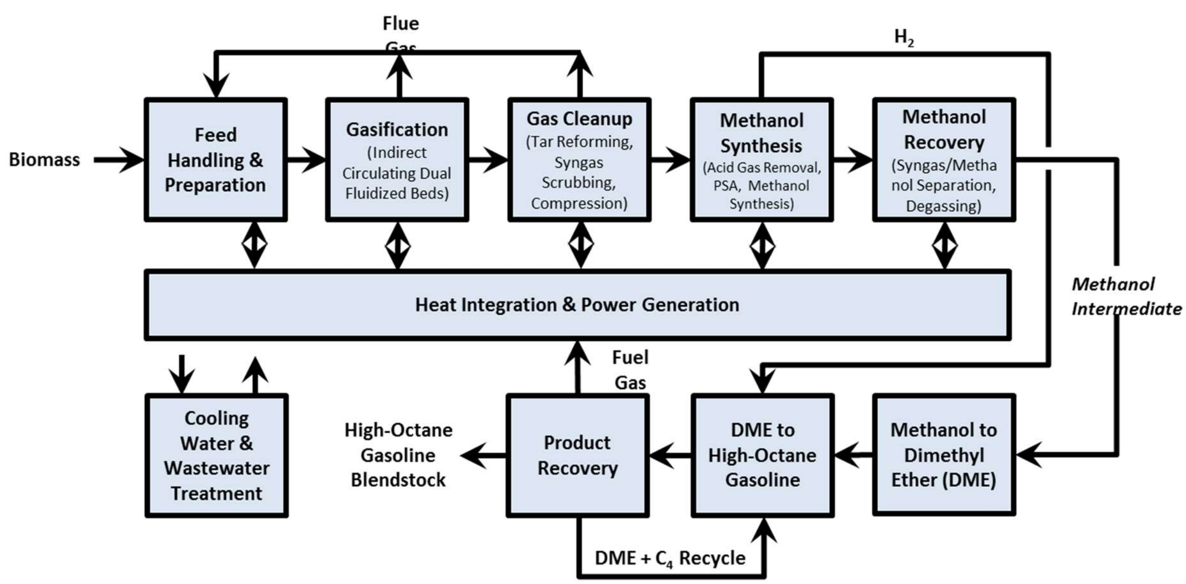


Figure 3 Process Flow Diagram for High Octane Gasoline via Indirect Liquefaction in the 2020 SOT (Harris et al. 2021)

Table 3 Key Indirect Liquefaction Process Parameters

	2021 SOT Value	Unit
HOG yield	6.0	MMBtu/dry ton feedstock
Surplus electricity	19	Btu/MMBtu of HOG
Diesel energy use	2,308	Btu/MMBtu of HOG
Char produced and combusted	779,711	Btu/MMBtu of HOG
Fuel gas produced and combusted	716,861	Btu/MMBtu of HOG
Magnesium oxide consumption	10.9	g/MMBtu of HOG
Fresh olivine consumption	443.0	g/MMBtu of HOG
Tar reformer catalyst consumption	7.9	g/MMBtu of HOG
Methanol synthesis catalyst consumption	3.8	g/MMBtu of HOG
DME catalyst consumption	7.3	g/MMBtu of HOG
Beta zeolite catalyst consumption	21.6	g/MMBtu of HOG
Zinc oxide catalyst consumption	2.0	g/MMBtu of HOG
LO-CAT chemicals	95.8	g/MMBtu of HOG
Dimethyl disulfide	1.7	g/MMBtu of HOG
Amine	3.5	g/MMBtu of HOG
Water consumption	28.0	gal/MMBtu of HOG

2.3.2 Sludge Hydrothermal Liquefaction (HTL)

HTL uses hot, pressurized water (e.g., 347°C and 20.5 MPa) in the condensed phase to convert biomass to a thermally stable oil product (also known as "biocrude"), which can then be thermocatalytically upgraded to hydrocarbon fuel blendstocks (Snowden-Swan et al. 2022). This technology has high carbon efficiency and can be applied to a wide range of wet feedstocks at similar processing conditions. The wet waste examined in the analysis is wastewater residuals (sludge) generated at water resource recovery facility (WRRF). The configuration includes an HTL plant co-located with a WRRF and a larger scale biocrude upgrading plant for producing hydrocarbon fuel blendstocks. The SCSA of this pathway considers fuel production processes starting from biocrude production (HTL plant) followed by biocrude upgrading to RD (upgrading plant), and RD transportation and combustion in vehicles, as shown in Figure 4.

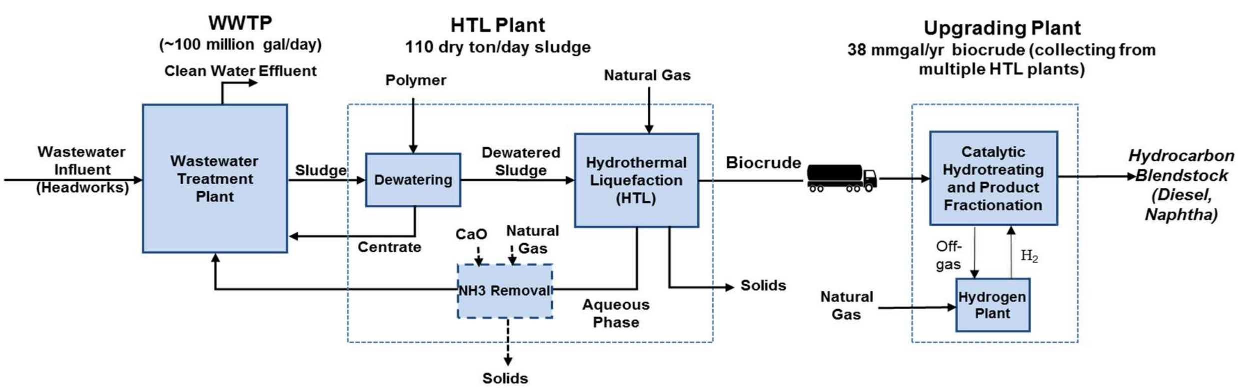


Figure 4 A Simplified Process Flow Diagram of the WRRF/HTL Plant and Centralized Biocrude Upgrading Plant Design

The operations at the HTL plant to produce biocrude and the subsequent biocrude upgrading operations in the 2021 SOT case remain the same. Table 4 summarizes major inputs and outputs of the HTL process for all the cases investigated. Table 5 presents the material and energy inputs and outputs of the upgrading plant.

Biocrude is assumed to be transported using trucks within a 100-mile radius to a large-scale centralized upgrading plant where it is converted to a hydrocarbon fuel blendstock.

Table 4 Energy and Material Balances (per lb of Biocrude Produced) at the HTL Plant

	Unit	With Ammonia Removal	Without Ammonia Removal
Material and Energy Inputs			
Dewatered sludge	(dry lb)	2.6	2.6
Natural gas	(Btu)	1,292	1,095
Electricity	(Btu)	309	294
Dewatering polymer	(lb)	0.012	0.012
Quicklime (CaO)	(lb)	0.113	0
Cooling water makeup	(gal)	0.0066	0.0066

Table 5 Material and Energy Inputs and Outputs, per MMBtu of Fuel Produced at the Upgrading Plant

	Unit	2021 SOT Case
Material and Energy Inputs		
Biocrude	lb	70.2
Natural gas	Btu	79,692
Electricity	Btu	10,287
Cooling tower chemical	g	0.3
Boiler chemical	g	0.2
Hydrotreating catalyst (CoMo/γ-Al_2O_3)	g	24.4
Hydrotreating catalyst (NiMo/γ-Al_2O_3)	g	3.9
Hydrocracking catalyst	g	0.2
Hydrogen plant catalyst (Ni)	g	0.3
Cooling water makeup	gal	5.4
Boiler feedwater makeup	gal	2.4

In order to evaluate the life-cycle GHG emissions associated with renewable diesel fuel, an energy allocation approach was applied in which GHG emissions are allocated between diesel (main product) and naphtha (co-product) based on their energy contents. The chemicals and catalysts required for the upgrading processes are incorporated into GREET to capture upstream energy use, emissions, and water consumption associated with their production. The production pathways of the materials listed in Tables 4 and 5 are available in GREET. Boiler chemical GHG emission burdens, however, were not included in the analysis because of lack of information.

The impact of excluding such chemicals would likely be small, given their very low consumption levels.

2.3.4 Biochemical Conversion

As in previous SOT cases, the biochemical conversion pathway to produce renewable hydrocarbon fuels (primarily in the diesel range) includes two approaches that utilize carboxylic acids and 2,3-butanediol (BDO) as fermentation intermediates in the 2021 SOT. In the SCSAs, we focused on the conversion scenario of both fermentation pathways that co-produce a significant amount of chemical co-product by upgrading the lignin stream, as well as recovering sodium sulfate salt from the wastewater treatment step, which could displace conventionally produced sodium sulfate. Other conversion scenarios that could burn the lignin to produce process heat and steam are also included here to understand the sustainability implications of such alternative designs.

Figure 5 is a high-level PFD of the biochemical conversion design with lignin-derived chemical co-production. The process remains largely the same as that reflected in the 2020 SCSA (Cai et al. 2021). In summary, the design consists of deacetylation and mechanical refining (DMR) pretreatment, followed by enzymatic hydrolysis to deconstruct biomass carbohydrates into monomeric sugars, which are subsequently upgraded through fermentation to either carboxylic acids or BDO intermediates. The respective fermentation intermediate product is recovered and sent through a series of catalytic reaction steps to be upgraded to hydrocarbon fuels. The liquor from the deacetylation (mild alkaline extraction) step is combined with the residual lignin and other hydrolysate solids downstream and subjected to further alkaline deconstruction before being routed through subsequent conversion steps to produce a co-product. A key update in the 2021 SOT reflects a switch from adipic acid as the selected coproduct (derived from lignin fermentation to muconic acid), to β-ketoadipate (BKA, a closely-related product which may be directly fermented from lignin monomers and ultimately destined for the same end-product market as adipic acid). Alternatively, the SOT also considers a case without lignin upgrading to co-products, where residual solid lignin is burned in the boiler and deacetylation black liquor is routed to wastewater treatment. The process utilizes substantial quantities of caustic (sodium hydroxide) and acid (sulfuric acid) across several processing steps. The resultant sodium sulfate salt is assumed to be recovered for sale as an additional minor co-product (alternative options may be investigated in the future to recover and recycle the caustic/acid chemicals internally, thus avoiding the large caustic/acid makeup demands and resultant sodium sulfate co-product recovery). The 2021 SOT maintains the use of a more optimal two-stage deacetylation step first incorporated in the 2020 SOT, first utilizing sodium carbonate, followed by standard sodium hydroxide deacetylation, which was found to enable better sugar yields while reducing sodium hydroxide demands by 70% via partial replacement with sodium carbonate (which is significantly more favorable both from a cost and GHG standpoint). Davis and Bartling (2022) provides more details on the process design, performance targets, and TEA results.

Given the significant amount of bioproduct co-product (BKA) and its significant impact on the sustainability results, we took three co-product handling methods (a purpose-driven, process-level allocation method, the displacement method, and the biorefinery-level analysis) to address the 2021 SOT case of the biochemical conversion pathway. Among these methods, the process-level allocation method allows us to separate the biorefinery inputs according to their purposes, namely, whether they are used for the fuel production, or used for the co-product production, or contribute to both. This ensures a plausible estimation of the sustainability impacts associated with different input streams that are purposefully contributing to different products.

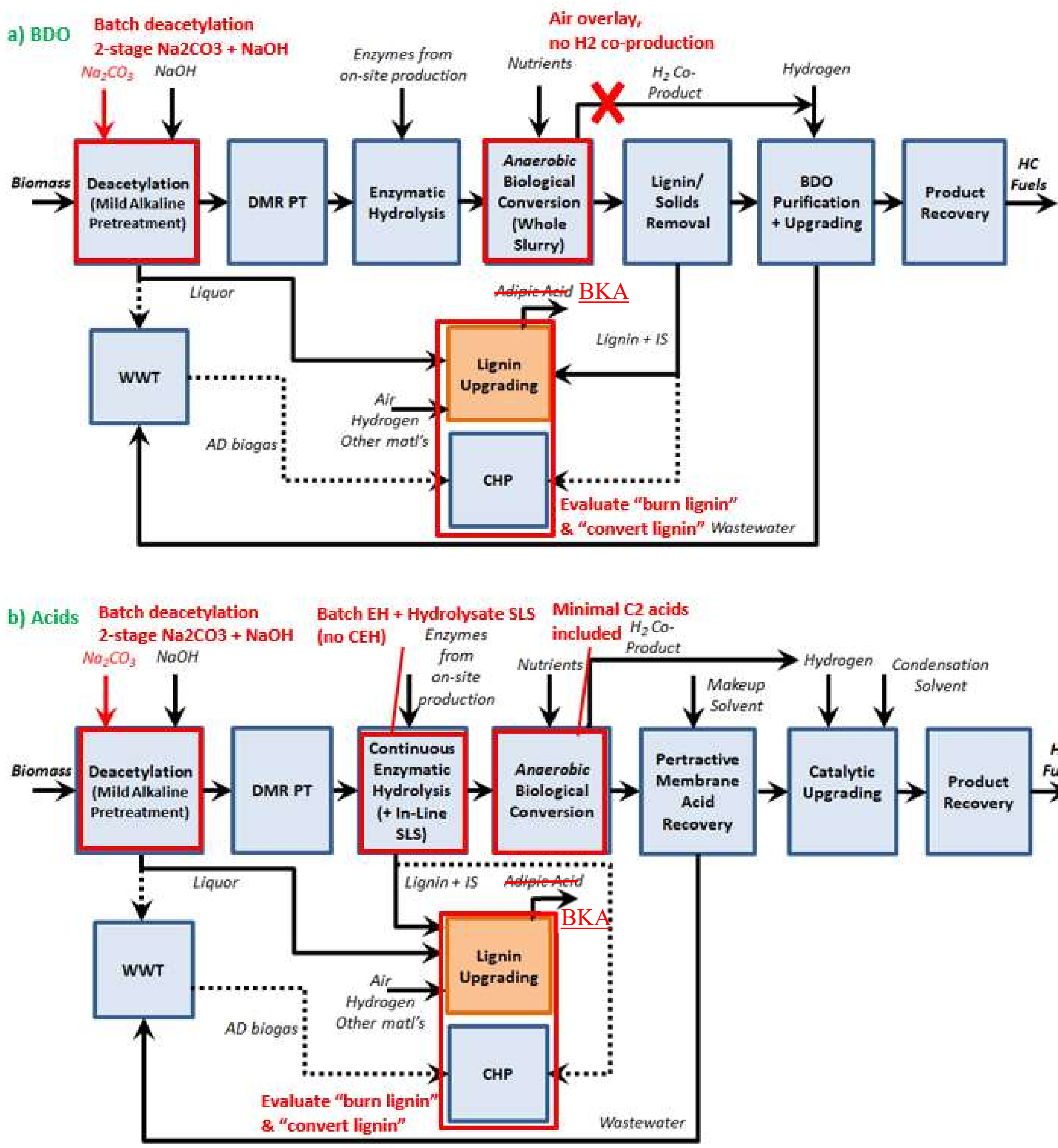


Figure 5 Process Flow Diagram of the Biochemical Conversion Design Case with Two Lignin Strategies: (1) Burn Lignin and (2) Convert Lignin to Co-Product. Modifications from the 2030 targets as reflected in the current 2021 SOT case are denoted in red (Davis et al. 2021)

With the purpose-driven, process-level allocation method, the inputs commonly shared by producing both the fuel and non-fuel products were allocated based on either the masses or the market values of the products. The mass-based yields of both products are informed by the process modeling, and the market prices for the renewable diesel and BKA are assumed to be $2.5/GGE and $0.85/lb, respectively.

Tables 6 presents the overall energy and material balances of the biochemical conversion pathway for both intermediate designs in the 2021 SOT case.

Table 6 Energy and Material Balances of the Biochemical Conversion Pathway for Both the Acids and BDO Intermediate Designs, 2021 SOT Case. Yellow inputs contribute to fuel production only, green inputs contribute to the biochemical production only, and blue inputs and outputs are shared by both the fuel and biochemical products.

	Via Acids		Via BDO		
	2021 SOT (Burn Lignin)	**2021 SOT (Convert Lignin – Base)**	**2021 SOT (Burn Lignin)**	**2021 SOT (Convert Lignin – Base)**	
Products	**Production Rate**				
Hydrocarbon fuel	9,833	9,815	10,851	10,882	kg/hr
	103	103	115	115	MM kcal/hr (LHV)
	410	409	455	457	MMBtu/hr
Co-Products					
Beta ketoadipate	0	1,991	0	1,968	kg/hr
Recovered sodium sulfate salt from WWT	10,304	14,639	10,581	13,810	kg/hr
Resource Consumption	**Flow Rate (kg/hr)**				
Biomass feedstock (20% moisture)	104,167	104,167	104,167	104,167	
Sulfuric acid, 93%	9,235	11,375	9,235	10,521	
Caustic (as pure)	2,000	4,280	2,000	3,582	
BKA train		2,280		1,582	
Both		2,000		2,000	
Sodium carbonate	6,667	6,667	6,667	6,667	
Ammonia	1,261	2,319	1,160	2,189	
Fuel train		62		62	
BKA train		17		17	
Both		2,240		2,110	
Glucose	1,312	1,312	1,312	1,312	
Corn steep liquor	1,226	1,226	918	918	
Corn oil	7	7	7	7	
Host nutrients	37	37	37	37	
Sulfur dioxide	9	9	9	9	

Table 6 (Cont.)

	Via Acids		Via BDO		
	2021 SOT (Burn Lignin)	2021 SOT (Convert Lignin – Base)	2021 SOT (Burn Lignin)	2021 SOT (Convert Lignin – Base)	
Diammonium phosphate	169	169	103	103	
Flocculant	407	407	435	436	
Toluene solvent makeup	90	90	0	0	
Hydrogen	0	0	868	865	
Boiler chemicals	0	0	0	1	
FGD lime	111	197	109	183	
WWT polymer	37	0	34	0	
Cooling tower chemicals	3	1	2	1	
Makeup water	330,952	262,876	119,427	150,469	
Natural gas for boiler	0	100	0	6,400	
Natural gas for hot oil system	39	39	0	0	MMBtu/hr
Grid electricity (net import)	7,019	56,869	23,768	41,073	kW
Fuel train		22,194		17,904	
BKA train		3,311		3,303	
Both		31,364		19,866	

About 97% of the toluene solvent makeup for the acids case ends up in the boiler and is combusted. The CO_2 emissions of toluene combustion are fully accounted for, and the emissions are considered fossil CO_2 emissions because toluene is made from fossil feedstock. CO_2 released upon acid neutralization of sodium carbonate (maintained in the 2021 SOT as part of the deacetylation step noted above) is also accounted for as fossil CO_2 emissions. Natural gas is used as a supplemental fuel in the boiler in the BDO intermediate route or in a hot oil heating system in the acids' intermediate route to meet process heat demands. Its use, as shown in Table 6, reflects the net gas inputs after accounting for burner efficiency losses. Grid electricity import is required for both fuel pathway designs, driven in part by high power/heat demands for the process and in part by diverting a portion of the residual solids (lignin) away from the boiler for BKA co-production.

2.3.5 Algae Hydrothermal Liquefaction (HTL)

This SCSA evaluates RD production from wastewater (WW)-grown algae in a water resource recovery facility (WRRF) system via HTL and biocrude upgrading.

Figure 6 displays a simplified PFD for the WRRF algae conversion via an HTL and upgrading system. Detailed process designs for growing algae in distributed WWTPs and transporting to an HTL biorefinery co-located with the largest WWRF for conversion and upgrading system to make renewable diesel and naphtha-range fuels are given in (Zhu et al. 2022).

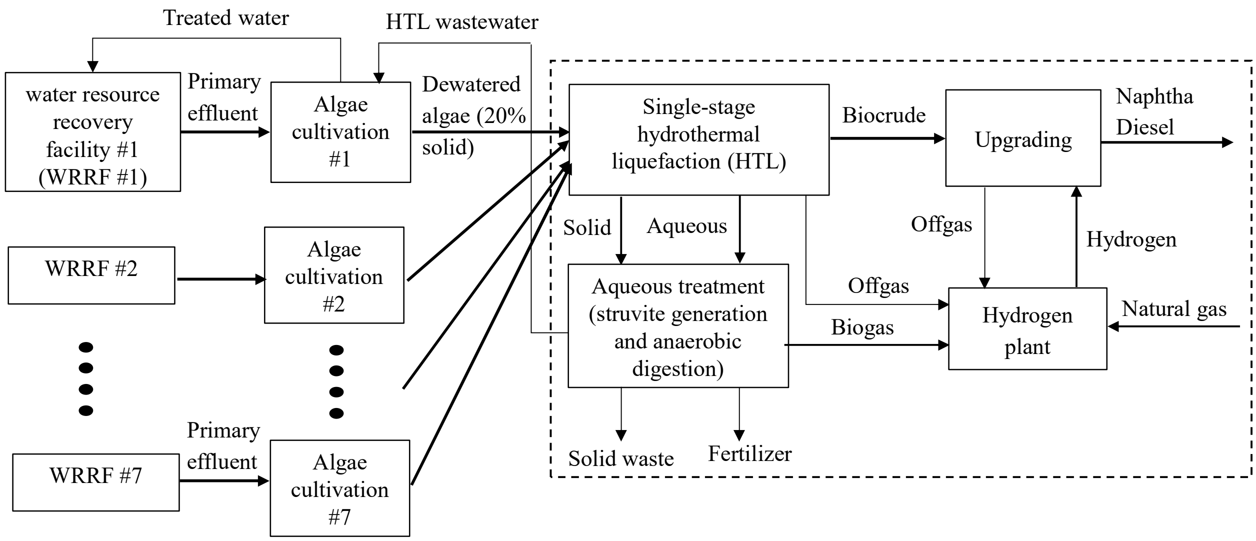


Figure 6 Process Flow Diagram for Hydrothermal Liquefaction of Wastewater Treatment Plant Algae for Renewable Diesel Production in the 2021 SOT

Nutrients in wastewater and CO_2 in air are the only nutrients source and the major carbon source for algae growth, respectively. Therefore no external carbon or nutrients are required. Power demand for cultivating the algae in the WRRF is entirely attributed to removing the nutrients from the wastewater in the WRRF. Hence, the WW-grown algae is considered a by-product and carries little material and energy burdens. Algae is harvested at 5% solid content at the algae cultivation unit in a WRRF, and dewatered to 20% solid content via centrifuge before being transported to the HTL biorefinery. Energy consumption for dewatering algae from 5% solids to 20% is modeled following NREL's algae farm model (Davis et al. 2016a).

The HTL biorefinery also produces struvite as a co-product, which can be used as a fertilizer. We account for the credits of struvite production using the displacement method, by assuming that struvite displaces synthetic nitrogen and phosphorus fertilizers.

As described in detail in Zhu et al. (2022), WW-grown algae was grown in the primary effluent from a WRRF. The production rate of algae per gallon wastewater, with seasonal variations, and the flow rates of primary effluents are used to specify the plant scale for the HTL conversion process. Wet storage was assumed in the 2021 SOT to store part of algae in summer/spring seasons with high algae production rates and used later in winter/fall to eliminate the seasonal algae productivity variation impacts on the conversion plant. The primary effluent for algae cultivation is assumed to be from the water reclamation plants in the greater Chicago area. The Metropolitan Water Reclamation District (MWRD) of Greater Chicago owns and operates one of the world's largest water reclamation plants (Stickney plant, located in Cicero, IL) and six other plants, with a combined treatment capacity of over 1 billion gallons of wastewater per day (MWRD 2021). As shown in Figure 7, the HTL plant is assumed to be a centralized plant and located closest to the largest WRRF in Cicero, the Stickney plant (see Figure 7, WRRF1). The algae from each WRRF in the greater Chicago area is transported to the HTL plant for processing. The average transportation distance is about 50 miles based on the radius of the circle with HTL in the center as shown in the figure. The proposed arrangement facilitates the transportation of algae from the largest WRRF to the conversion facility and the recycle of the aqueous stream from HTL to a nearby WRRF algae cultivation unit.

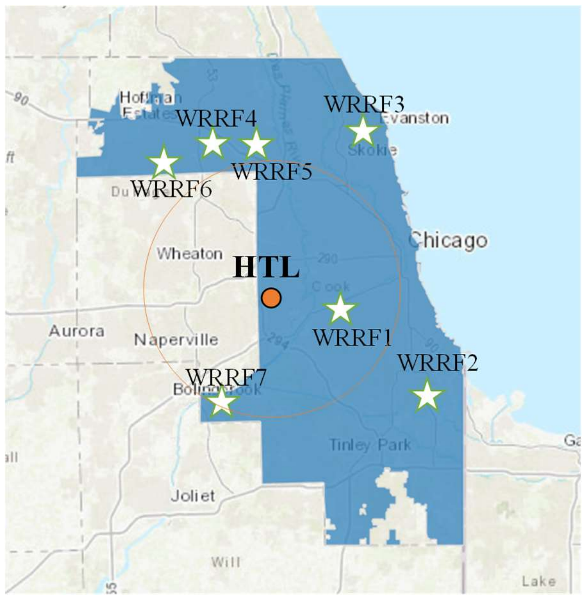


Figure 7 WW-grown algae HTL conversion plant scenario assumed for the SOT case

Table 7 lists the overall material, energy, and water consumption for the modeled HTL conversion process at the plant in the 2021 SOT case.

Table 7 Material, Energy, and Water Consumption for the Modeled HTL Conversion and Upgrading Process, 2021 SOT Case.

	Values	Unit
Fuel Products		
Diesel	841	kg/h
	35	MMBtu/h
Naphtha	351	kg/h
	15	MMBtu/h
Co-product and byproduct		
Struvite	2,019	kg/h
Resource Consumption		
Algae (AFDW basis), annual average	5,237	kg/h
Sulfuric-Acid (96 wt% pure) makeup	511	kg/h
MgO	202	kg/h
$MgCl_2$	201	kg/h
Hydrotreating main bed catalyst	0.3	kg/h
HT guard bed catalyst	1.6	kg/h
Natural gas for H_2 generation	176	kg/h
Natural gas for summer drying	0	kg/h
Process water makeup	12,090	kg/h
Purchased Electricity	724	kW

2.3.6 Combined Algae Processing (CAP)

The CAP model is based on NREL’s documented framework involving low-temperature biochemical fractionation of algal biomass into its respective constituents (lipids, carbohydrates, and protein) for subsequent upgrading of each constituent to fuels or products (Wiatrowski et al. 2022). In the process configurations evaluated here, a saline algae CAP model is configured to produce renewable fuels from lipids via extraction and upgrading and from sugars via either acid or BDO fermentation intermediates in the SOT and target cases (similar to the sugar fermentation concepts discussed previously for biochemical conversion). Protein and other residual fractions are routed to anaerobic digestion for combined heat and power generation as well as nutrient recycle credits back to the cultivation stage. As in the 2020 SOT, a polyurethane (PU) co-product is produced from a fraction of the extracted algal lipids via epoxidation and ring opening to polyols, followed by reaction with isocyanates to produce PU foam (in part based on data furnished by UCSD under separate BETO project support). Figure 8 shows a block-flow diagram of the CAP conversion process. The 2021 SOT case reflects minor updates in the SOT algae farm model cultivation performance parameters, with other process parameters maintained consistently with the 2020 SOT.

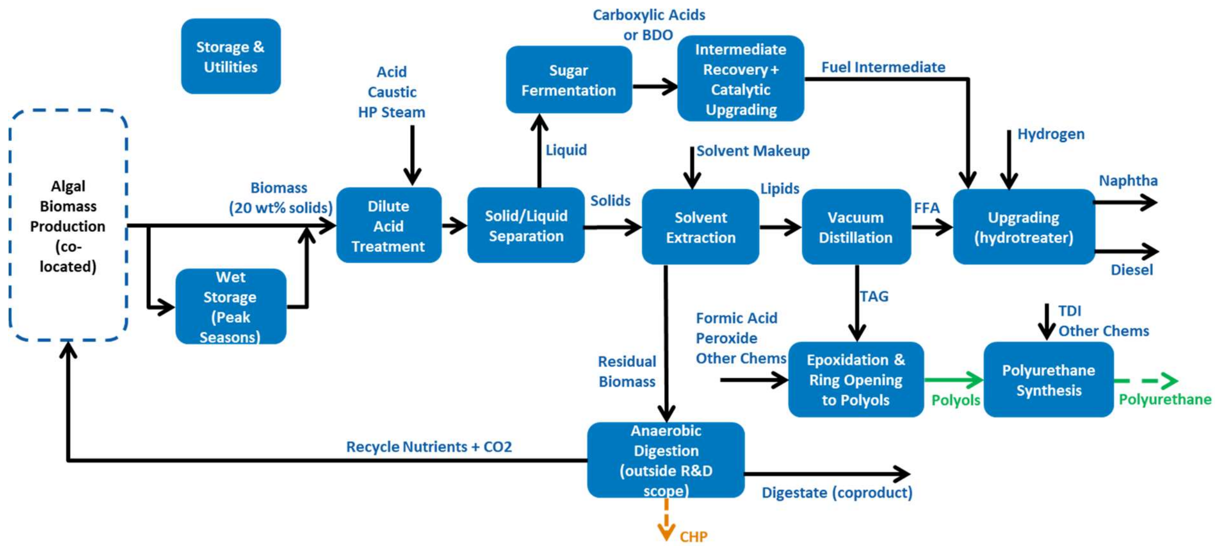


Figure 8 Block-Flow Diagram of the CAP Conversion Process as Reflected in the 2021 SOT

Given the significant amount of PU co-product as maintained in the 2021 SOT case, which accounts for 54% by mass of the total product slate including RD, naphtha, and PU, we applied the same purpose-driven, process-level allocation method in this SCSA. For the inputs that are commonly shared by production of both the fuel and non-fuel products, we apply an allocation method based on either the masses or the market values of both products. The mass-based yields of both products are informed by the process modeling, and the market prices for the hydrocarbon fuels and PU are assumed to be $2.5/GGE and $2.04/lb. We also allocate the surplus electricity that is generated from the entire conversion process between the fuel and non-fuel products. The surplus electricity accounts for about 14% of the total energy products by energy content. We apply the displacement method to evaluate its sustainability impacts. At the same time, we apply an energy-based allocation method to allocate emission burdens between both liquid transportation fuels, the renewable diesel and the naphtha fuel products.

To address the effects of the significant output of the PU co-product, we applied the purpose-driven, process-level allocation method to address the 2021 SOT case in addition to the displacement method and biorefinery-level analysis. The environmental impacts, including GHG emissions, water consumption, and NO_x emissions, of conventional, fossil-derived flexible PU foam were model in GREET (Keoleian et al. 2012) and used to account for the displacement credit and biorefinery-level emissions.

Table 8 lists the overall energy and material inputs for the modeled CAP conversion process in the 2021 SOT case, via either acids or BDO intermediate pathways for fuel production.

Table 8 Overall Energy and Material Inputs and Outputs in the Modeled CAP Conversion Processes in the 2021 SOT Case via Acids and BDO as Intermediate Pathways. Yellow inputs contribute to fuel production only, green inputs contribute to the biochemical production only, and blue inputs and outputs are shared by both the fuel and biochemical products.

	Via Acids	Via BDO	
Products	**Production Rate**		
Hydrocarbon Fuel			
Diesel	2,065	1,860	kg/hr
Naphtha	811	1,002	kg/hr
Co-products			
Polyurethane	3,318	3,318	kg/hr
Power exported to grid	5,580	5,678	kW
Resource Consumption	**Flow Rate (kg/hr)**		
Feedstock (AFDW basis)	14,727	14,727	
Pretreatment			
Sulfuric acid (93% pure)	1,304	1,304	
Ammonia	421	421	
Lipid Extraction and Cleanup			
Hexane requirement	77	78	
Ethanol	31	31	
Phosphoric acid (oil cleanup)	42	42	
Silica (oil cleanup)	4	4	
Clay (oil cleanup)	8	8	
Carboxylic Acid / 2,3-BDO Conversion			
Corn steep liquor	669	99	
Diammonium phosphate	70	12	
Hydrogen		76	
Flocculant	59	59	
Dehydration catalyst		0.06	
Oligomerization catalyst		0.1	
Hydrotalcite	1		
Hexane	1		
Final Fuel Upgrading (HDO/HI)			
Hydrogen	97	87	
One-step HDO/HI catalyst (1% Pt/SAPO-11)	0.2	0.2	
Polyurethane Production			
Formic acid	320	320	
H_2O_2	507	507	
Catalysts and other chemicals	9	9	
Nitrogen	48	48	
Toluene diisocyanate	880	880	
Diethanolamine	9	9	
Surfactant	16	16	

Table 8 (Cont.)

	Via Acids	Via BDO
Other Resource Consumption		
Supplemental natural gas (total)	1,850	3,079
Supplemental natural gas (fuel+PU)	912	1,266
Supplemental natural gas (fuel)	101	694
Supplemental natural gas (PU)	837	1,120
Process water (total)	59,606	95,525
Process water (fuel+PU)	43,020	49,658
Process water (fuel)	91	29,372
Process water (PU)	16,495	16,495
Output Streams	**Flow Rate (kg/hr)**	
AD digestate cake (dry basis total flow)	3,398	3,231
AD digestate cake bioavailable N	17	16
AD effluent NH_3	210	204
AD effluent DAP	102	72
Recycle water (excluding N/P nutrients)	95,794	98,151
CO_2 Recycle		
CO_2 (biogenic)	8,460	8,338
CO_2 (fossil)	5,595	8,967

A nutrient-rich effluent produced in the AD process can be recycled to the algae cultivation ponds. For the SCSAs, we assumed that the NH_3 and DAP from the AD effluent reduce the nitrogen and phosphorus demand (as indicated by the algal farm model) and the bioavailable nitrogen from the AD digestate cake is sold as a nitrogen fertilizer and displaces synthetic nitrogen fertilizers on a kg for kg basis.

3 RESULTS AND DISCUSSION

The feedstock and conversion process model input/output inventories were furnished to the GREET model to calculate overall life-cycle metrics of the five renewable fuel pathways.

3.1 Indirect Liquefaction

The SCSA of the IDL pathway used a 50-50 blend of clean pine and logging residue in the 2021 feedstock SOT.

3.1.1 Supply Chain Greenhouse Gas Emissions

The supply chain GHG emissions of HOG via IDL is 18.1 g CO_2e/MJ in the 2021 SOT case. Clean pine production and biomass logistics are the dominant contributors to the supply chain GHG emissions, accounting for 26% and 59% of the supply chain GHG emissions, respectively. The IDL conversion process contributes 10% of the supply chain GHG emissions. The GHG emission intensity of HOG production in the biorefinery is about 1.8 g CO_2e/MJ in the 2021 SOT case. Note that these conversion GHG emissions include both direct emissions from the combustion of intermediate process energy, such as biochar and fuel gas during the conversion stage, and upstream emissions associated with the production of catalysts used in the conversion. The energy self-sufficient design of the IDL conversion processes has contributed to the low emission intensity at the conversion step since the earlier SOT cases. With little contribution from energy consumption to GHG emissions from the IDL process, the production and use of catalysts is the major driver for the minimal GHG emissions from this supply chain step. Combustion of the fuel gas and char would produce CH_4 and N_2O, and these emissions are estimated through the application of emission factors in the GREET model developed for boiler combustion of refinery fuel gas and char. The 2021 SOT case has no co-product. Figure 9 shows the supply chain GHG emissions.

Compared with petroleum-derived gasoline, HOG via IDL offers a significant supply chain GHG emission reductions of 81% in the 2021 SOT case.

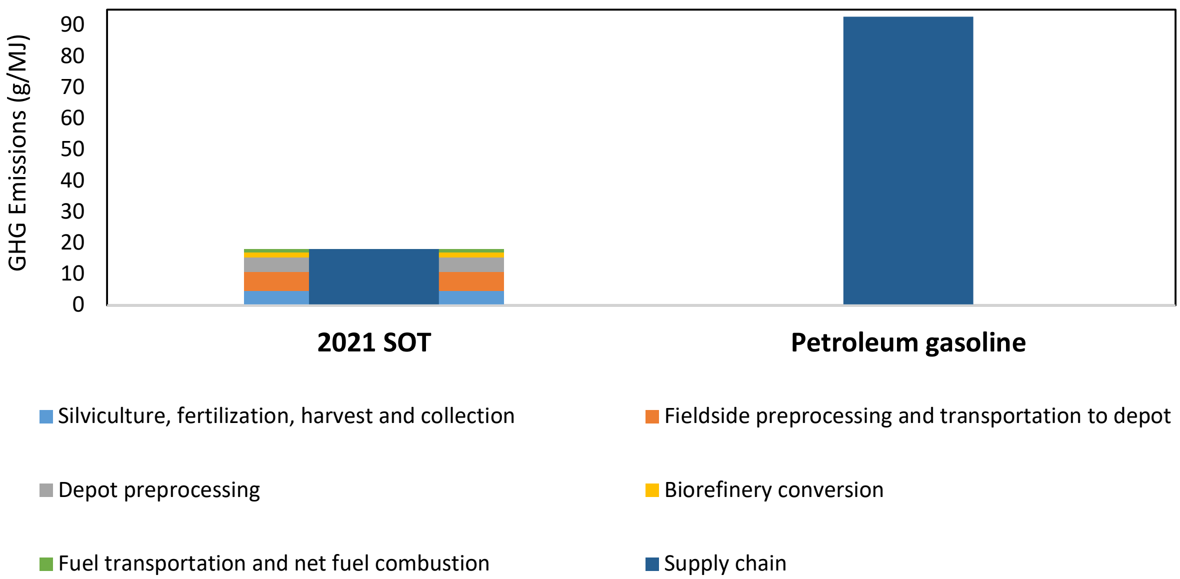


Figure 9 Supply Chain GHG Emissions (g CO_2e/MJ), High Octane Gasoline via IDL

At the biorefinery level with the minimal amount of co-produced electricity, essentially the biorefinery-level emission reduction comes entirely from HOG, as shown in Figure 10. About 473 kg CO_2e of GHG emission reduction could be achieved per ton of feedstock blend converted to HOG fuel via the IDL pathway.

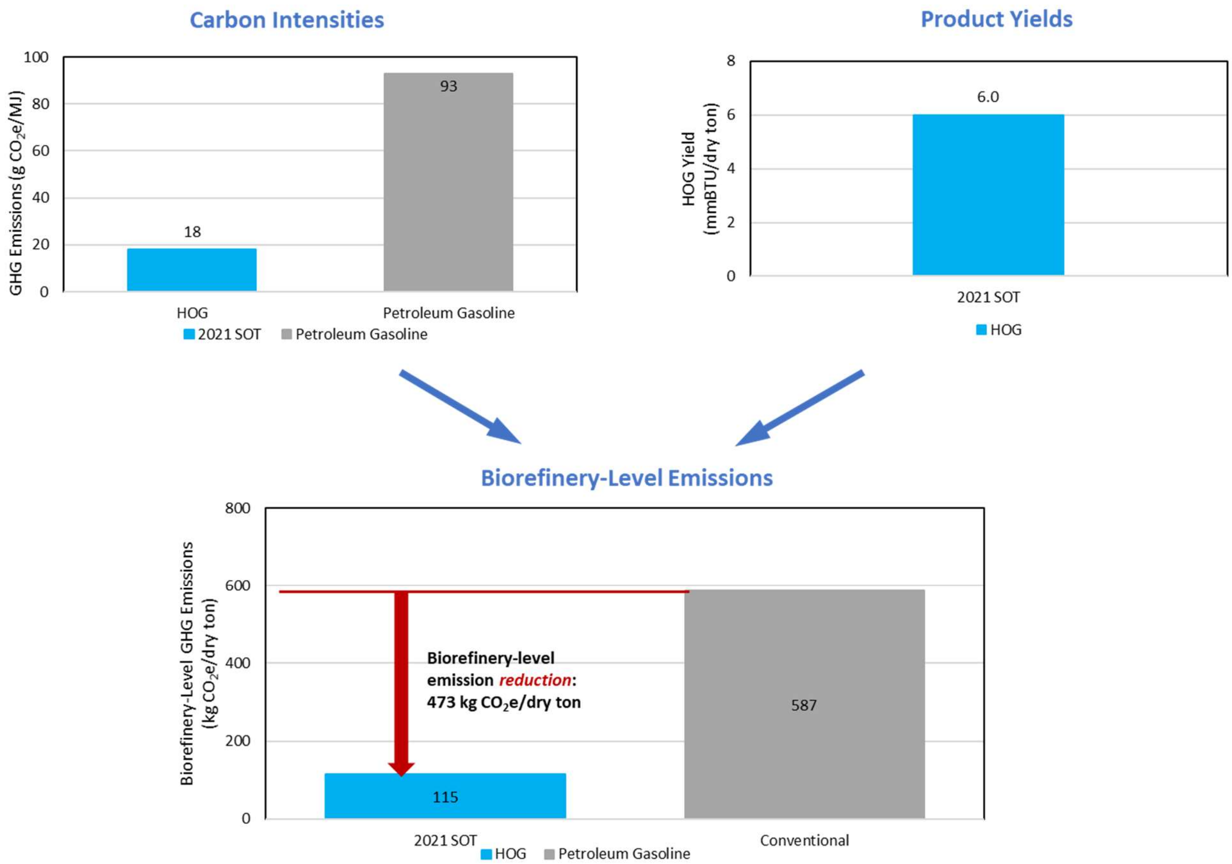


Figure 10 Biorefinery-Level Greenhouse Gas Emissions and Reductions, the 2021 SOT Case of the IDL Pathway

3.1.2 Supply Chain Water Consumption

The supply chain water consumption of HOG produced via IDL is about 4.8 gal/gasoline gallon equivalent (GGE) in the 2021 SOT case, compared to about 3.2 gal/GGE for petroleum gasoline blendstock (Wang et al. 2021).

Figure 11 shows the supply chain water consumption of HOG via IDL in gal/GGE. The largest contributor to the supply chain water consumption is the IDL process (i.e., biorefinery), accounting for about 70%. The water is consumed for process cooling and boiler feed water makeup. Another step contributing to the supply chain water consumption is the relatively energy-intensive depot preprocessing, accounting for about 20%, primarily owing to water consumption associated with the production of process energy (electricity) required for the preprocessing.

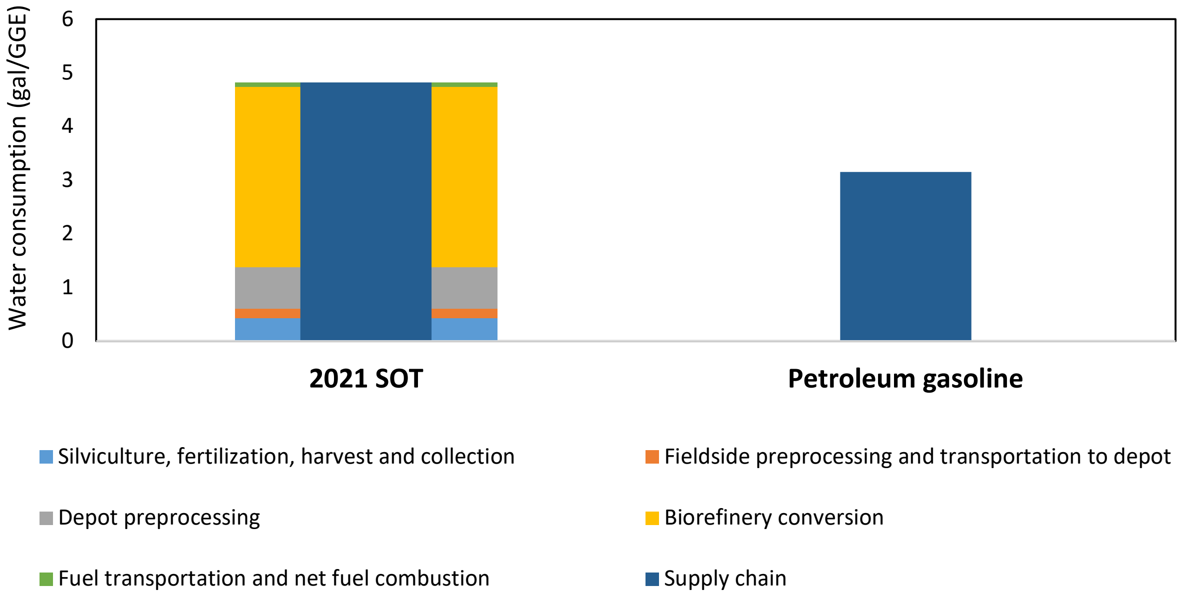


Figure 11 Supply Chain Water Consumption (gal/GGE) of High Octane Gasoline via IDL, Compared to 3.2 gal/GGE for Petroleum Gasoline

The direct water consumption during the conversion process remains about the same in the 2021 SOT case, which is 3.3 gal/GGE, as that in the 2020 SOT case.

3.1.3 Supply Chain NO_x Emissions

The supply chain NO_x emissions of HOG produced via IDL is about 0.16 g/MJ in the 2021 SOT case, compared to about 0.05 g/MJ for petroleum gasoline blendstock (Wang et al. 2021).

Figure 12 shows that NO_x emissions are mostly attributable to the IDL process, fieldside preprocessing, and biomass transportation. Similar to the other cases, combusting intermediate bio-char and fuel gas in boilers inside the biorefinery for process heat purposes is the dominant cause for the conversion NO_x emissions, accounting for about 69% of the total supply chain emissions. Fuel transportation by diesel truck and fuel combustion contributes about 0.02 g/MJ of the total supply chain emissions. Given the energy self-sufficient design of the IDL process, which heavily relies on the combustion of intermediate bio-char and fuel gas to meet process heat demand, NO_x emission control of this combustion source presents the greatest opportunity to mitigate the supply chain NO_x emissions of the HOG via IDL pathway.

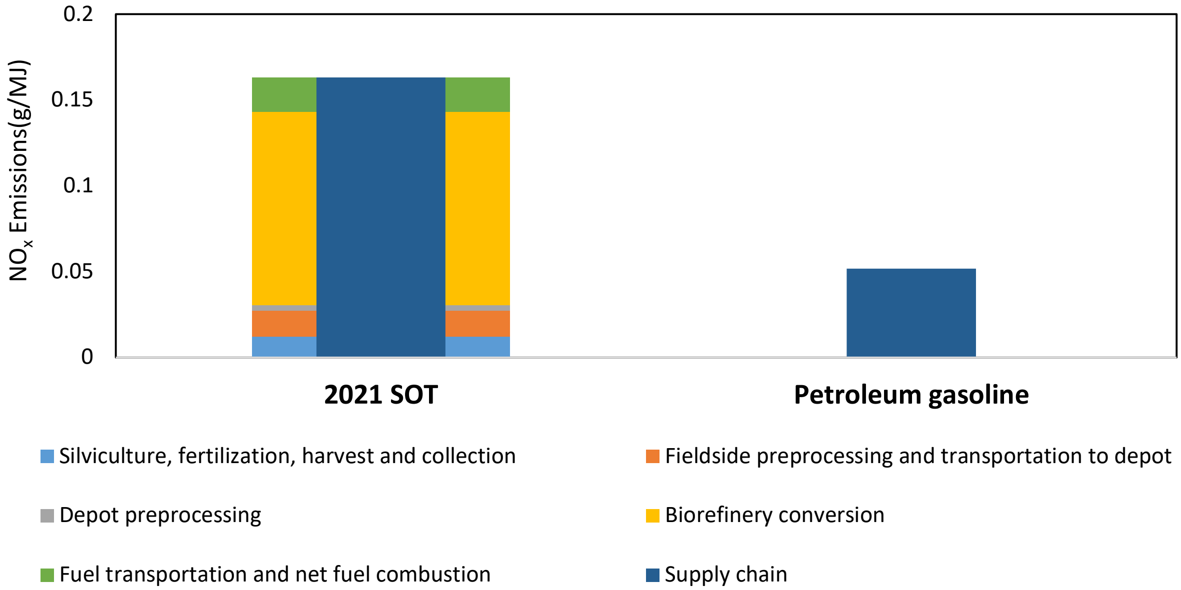


Figure 12 Supply Chain NO_x Emissions (g/MJ), High Octane Gasoline via IDL, Compared to 0.05 g/MJ for Petroleum Gasoline

3.1.4 Summary of Sustainability Metrics

Table 9 summarizes supply chain sustainability metrics in different functional units evaluated for the 2021 SOT case of HOG via IDL. In addition to GHG emissions, water consumption, and total NO_x emissions as described above, Table 9 lists the supply chain fossil energy consumption and the net energy balance (NEB) as two energy-related metrics. Fossil energy consumption of HOG via IDL shows a significant reduction of 83% in the 2021 SOT case, compared with that of petroleum gasoline, owing mostly to energy self-sufficient IDL process and the use of excess waste heat from the IDL process for feedstock drying, which reduces the need for external energy. NEB is defined as the balance of biofuel energy output minus the supply chain fossil energy consumption used to produce the biofuel. NEB represents the net fossil energy savings from using biofuels to displace fossil fuels. A net energy balance of 0.79 MJ/MJ of HOG produced is estimated for the 2021 SOT case, showing significant fossil energy saving benefits for HOG via IDL.

Table 9 Supply Chain Sustainability Metrics for High Octane Gasoline via IDL

	2021 SOT	Petroleum Gasoline
	Biofuel yield	
Million Btu/dry ton	6.0	
	Fossil energy consumption	
MJ/MJ	*0.21 (-83%)*	1.23
	Net energy balance	
MJ/MJ	0.79	
	GHG emissions	
g CO_2e/MJ	*18 (-81%)*	93
g CO_2e/GGE	2,214	11,357
	Water consumption	
gal/MJ	0.039	0.026
gal/GGE	4.8	3.2
	Total NOx emissions	
g NO_x/MJ	0.16	0.052
g NO_x/GGE	20.0	6.3
	Urban NOx emissions	
g NO_x/MJ	0.014	0.023
g NO_x/GGE	1.8	2.8

Note: The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

As air pollutant emissions (including NO_x emissions) are known to pose potential human health impacts, we define the emissions that occur in municipal statistical areas (MSAs) where more people could be exposed to the emissions as urban emissions, as differentiated from the total supply chain NO_x emissions regardless of where they occur. HOG via IDL shows about 37% reduction potential in urban NO_x emissions in the 2021 SOT case, compared with those of petroleum gasoline, because biorefinery and depot preprocessing emissions, the primary emission sources of HOG, are assumed to occur in rural, non-MSA areas where the biorefinery likely would be built.

3.2 Sludge Hydrothermal Liquefaction

The SCSA of the 2021 SOT case of the sludge hydrothermal liquefaction pathway incorporated two treatment scenarios for the conversion of sludge to biocrude via the HTL process: scenario 1 with ammonia removal from the HTL aqueous phase, and scenario 2 without ammonia removal from the HTL aqueous phase.

3.2.1 Supply Chain Greenhouse Gas Emissions

Figure 13 represents the supply chain GHG emissions and their key contributing supply chain processes in g CO_2e/MJ of RD produced from sludge via the HTL and upgrading processes. The GHG emissions reduction of the 2021 SOT case is compared with a life-cycle carbon intensity of 91 g CO_2e/MJ for petroleum diesel. The supply chain GHG emissions for the 2021 SOT case are lower than those for petroleum diesel, especially in the scenarios without NH_3 removal. In the scenario with NH_3 removal, RD GHG emissions represent a 78% reduction compared with petroleum diesel. When NH_3 is not removed from the HTL aqueous, RD GHG emissions represent an 83% reduction in the 2021 SOT case compared with petroleum diesel. Higher GHG emissions reductions when NH_3 is not removed are achieved by avoiding quicklime (CaO) use and reducing the use of the natural gas associated with the NH_3 stripping process. However, the WRRF would need to treat the additional NH_3 if it were not removed at the HTL plant.

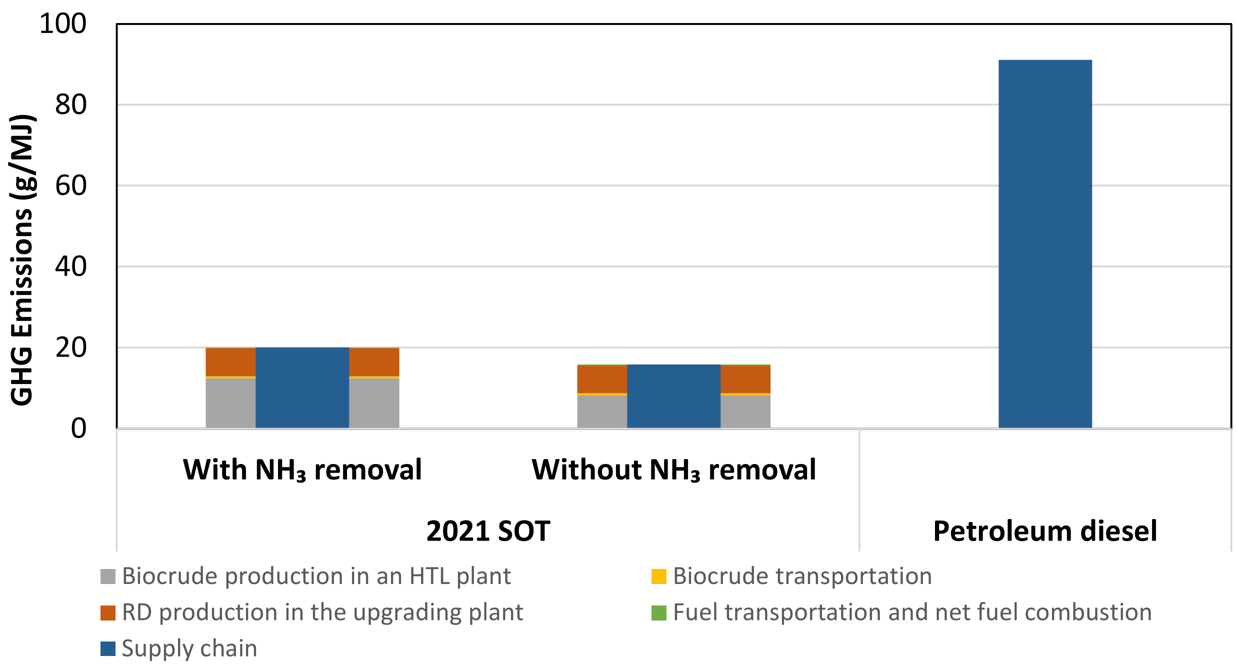


Figure 13 Supply Chain GHG Emissions (g CO_2e/MJ) of Renewable Diesel via Sludge HTL, Compared to 91 g CO_2e/MJ for Petroleum Diesel

The major contributor to the supply chain GHG emissions are the emissions during biocrude production in the HTL plant, accounting for about 62% of the total emissions with NH_3 removal, and for about 52% of the total emissions without NH_3 removal. When the HTL aqueous

NH_3 is not removed, the supply chain GHG emission intensities are lowered by about 4 g CO_2e/MJ in the 2021 SOT case.

It is worth noting that we started to consider the potential impacts of lime sludge that is formed during the ammonia stripping process to treat the HTL aqueous waste. Lime sludge is rich in $CaCO_3$. We assume that this solid waste is transported to a landfill by truck. The carbon in the lime sludge originates from the wastewater sludge and thus we assume that it is biogenic carbon. We assume that 49.2% of the biogenic carbon in the lime sludge upon soil amendment or landfill ends up as biogenic CO_2 emissions (0.216 g CO_2/g $CaCO_3$) (Cai, Wang, and Han 2014), while the remaining will be sequestered and result in a biogenic carbon sequestration credit of -0.224 g CO_2/g $CaCO_3$, which translates to about -1.4 g CO_2e/MJ of RD.

At the biorefinery level, without a biochemical co-product the biorefinery-level emission reduction comes entirely from the fuels (Figure 14). Approximately 837 kg to 887 kg CO_2e of GHG emission reduction could be achieved per ton of biosolids in wastewater sludge converted to renewable diesel via the HTL pathway, depending on whether ammonia removal is considered.

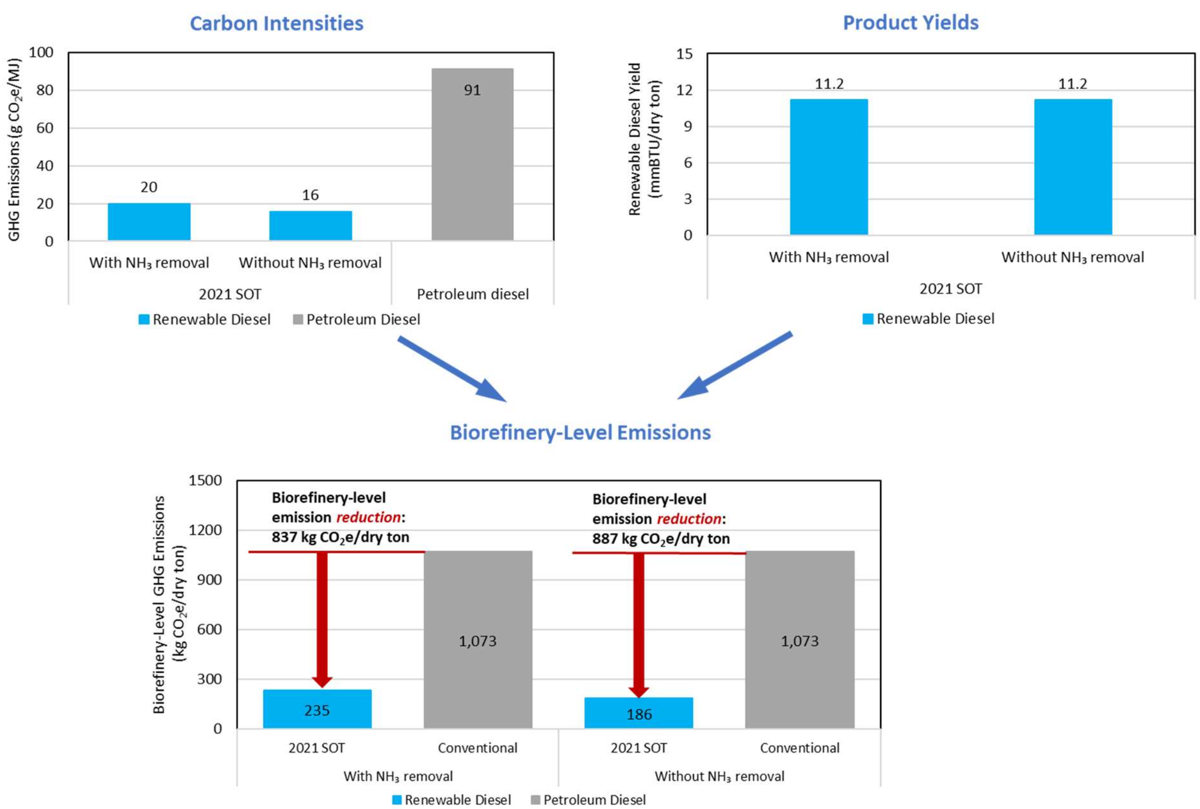


Figure 14 Biorefinery-Level Greenhouse Gas Emissions and Reductions, the 2021 SOT Case of the Wastewater Sludge HTL Pathway, with and without Ammonia Removal

3.2.2 Supply Chain Water Consumption

Figure 15 shows supply chain water consumption producing one GGE of RD from sludge via the HTL and upgrading processes. The 2021 SOT "with NH_3 removal" scenario consumes 2.3 gal/GGE, compared to 2.7 gal/GGE for petroleum diesel. When ammonia stripping is not part of the process design, water use during the conversion of sludge to biocrude is reduced to 1.8 gal/GGE, owing to the avoidance of embedded water consumption of CaO and reduction in electricity and natural gas consumption.

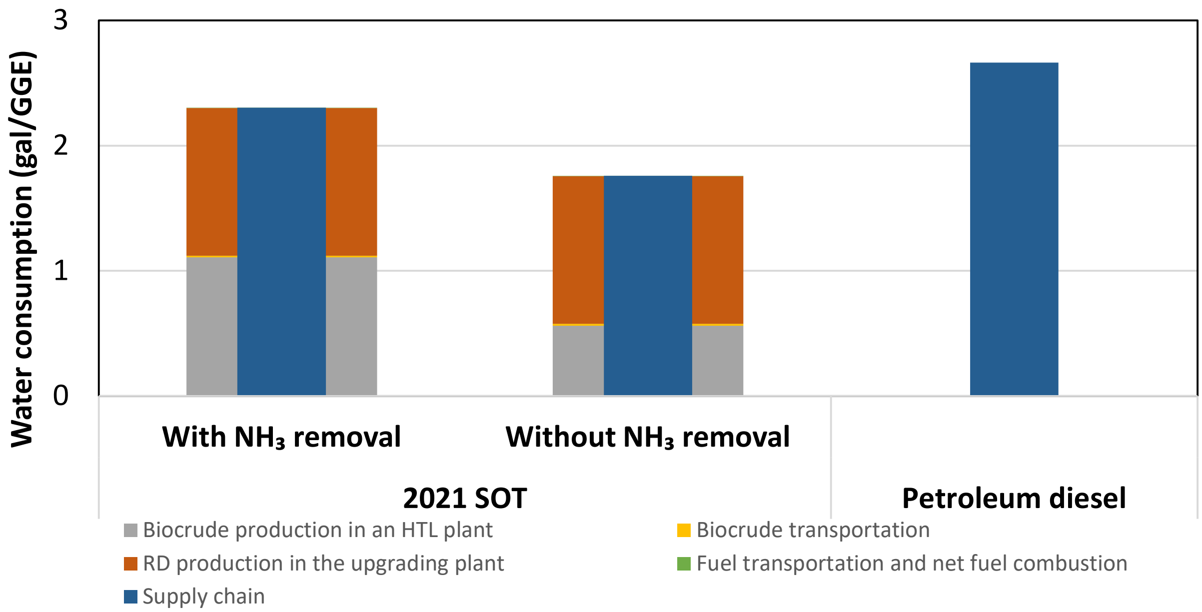


Figure 15 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via Sludge HTL, Compared to 2.7 gal/GGE for Petroleum Diesel

The direct water consumption during the conversion process in the 2021 SOT case remains the same as that in the 2020 SOT case, which is about 1.0 gal/GGE.

3.2.3 Supply Chain NO_x Emissions

Figure 16 shows that, in the 2021 SOT case, total supply chain NO_x emissions measure about 0.040 and 0.038 g/MJ with and without NH_3 removal, respectively. Fuel combustion represents the main contributor of NO_x emissions, which is assumed to equal that of petroleum diesel combustion, as modeled in GREET. The second-largest contributor is NO_x emissions associated with energy consumption during biocrude production.

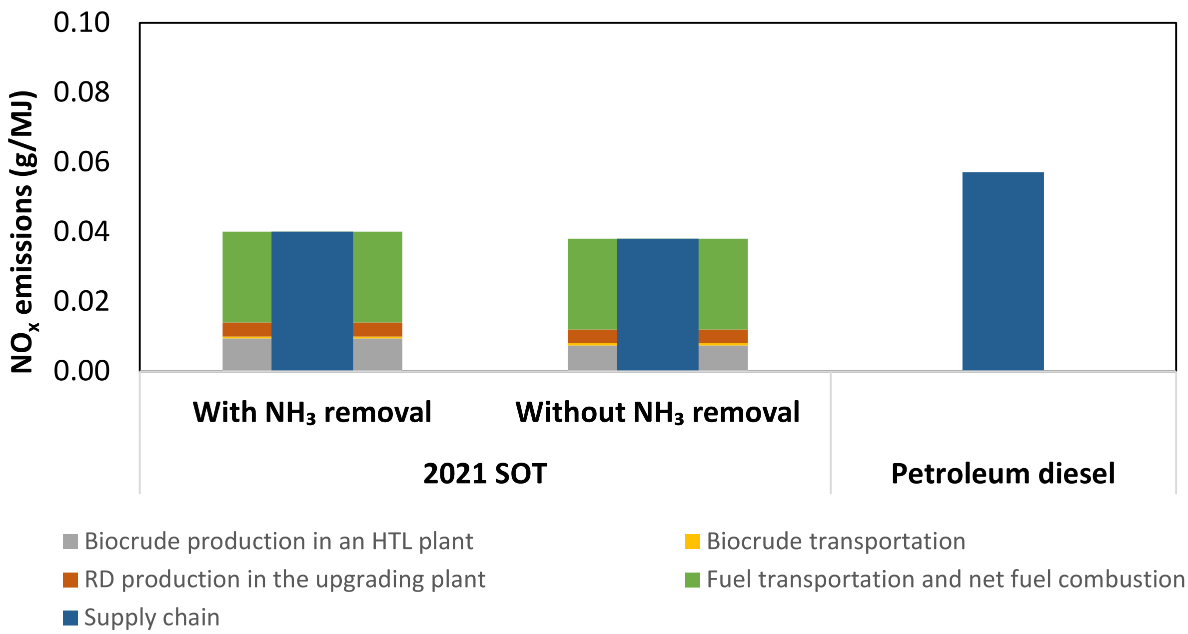


Figure 16 Supply Chain NO_x Emissions (g/MJ) of Renewable Diesel via HTL, Compared to 0.06 g/MJ for Petroleum Diesel

3.2.4 Summary of Sustainability Metrics

Table 10 summarizes the SCSA sustainability metrics evaluated for the 2021 SOT case of RD production from wet sludge via the HTL and upgrading processes. The supply chain fossil energy consumption of the 2021 SOT cases is 0.27 and 0.24 MJ per MJ of RD, with and without NH_3 removal, respectively, which is attributable to natural gas and electricity consumption in the HTL and upgrading processes. The NEB of RD is 0.73 MJ/MJ (with NH_3 removal) and 0.76 MJ/MJ (without NH_3 removal) for the 2021 SOT case of the sludge HTL pathway.

In the 2021 SOT case, the sludge HTL pathway shows a reduction in urban NO_x emissions by about 27% and 28% with and without NH_3 removal, respectively, compared with that of petroleum diesel.

Table 10 Supply Chain Sustainability Metrics for Renewable Diesel via Sludge HTL

	2021 SOT		
	With NH_3 removal	Without NH_3 removal	Petroleum Diesel
	Biofuel yield		
Million Btu/dry ton	11.2	11.2	
	Fossil energy consumption		
MJ/MJ	0.27	0.24	1.2
	Net energy balance		
MJ/MJ	0.73	0.76	
	GHG emissions		
g CO_2e/MJ	20 (*-78%)*	16 (*-83%)*	91
g CO_2e/ GGE	2,448	1,936	11,157
	Water consumption		
L/MJ	0.07	0.05	0.09
gal/GGE	2.3	1.8	2.7
	Total NO_x emissions		
g NO_x/MJ	0.040	0.038	0.057
g NO_x/GGE	4.9	4.7	7.0
	Urban NO_x emissions		
g NO_x/MJ	0.020	0.020	0.028
g NO_x/GGE	2.4	2.4	3.3

Note: The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

3.3 Biochemical Conversion

The SCSA of the biochemical pathway incorporated the 2021 SOT case of herbaceous feedstock with the 2021 SOT case of the biochemical conversion pathways via acids and BDO intermediates.

We use three co-product handling methods to derive supply chain GHG emission results of the biochemical conversion pathway when the lignin is upgraded to BKA:

1) Purpose-driven, process-level allocation method
2) Displacement method
3) Biorefinery-level analysis

The process-level allocation method separates process-level energy and material requirements between biofuel production and co-product production, and generates product-specific results for the biofuel and non-fuel co-product, respectively. The displacement method results for the biofuel combine effects of both the fuel and non-fuel co-product, and thus need to be interpreted with caution (Cai et al. 2018). The biorefinery-level results include emission reduction benefits of both the fuel product and the non-fuel co-product in comparison to the same amounts of the same products produced through conventional means from fossil feedstocks, thus presenting a complete picture of the biorefinery's emission performance.

3.3.1 Supply Chain Greenhouse Gas Emissions

Figure 17 displays the supply chain GHG emissions and their key contributing supply chain processes, in g CO_2e/MJ of RD, in the 2021 SOT case, compared with a life-cycle carbon intensity of 91 g CO_2e/MJ for petroleum diesel. The table presents results for two conversion process designs that 1) burn the lignin to generate heat and power for use by the conversion process or 2) convert and upgrade the lignin to BKA. When lignin is upgraded to BKA, we apply both mass- and market-value-based process-level allocation methods to allocate inputs that are common to both the fuel and BKA products. Feedstock preprocessing accounts for 6%-8% of the emissions in the 2021 SOT case when lignin is upgraded to BKA due to electricity and diesel usage for meeting feedstock quality targets for conversion. In both process designs, the conversion step is the major GHG emission source of the entire supply chain.

Where lignin is upgraded to BKA, large quantities of process chemicals are consumed at the DMR pretreatment step. These chemicals are responsible for a significant amount of GHG emissions. The recovered sodium sulfate salt from WWTP translates to a displacement emission credit of about 4 – 5 g CO_2e/MJ in both routes after the process-level allocation. GHG emission intensity of the fuel in the lignin upgrading to the BKA case is somewhat higher than that in the burning lignin case for both scenarios because additional NG and electricity are required when lignin is not burned to provide process energy for the biorefinery. The overall net GHG emission intensities of the fuel in the lignin conversion to BKA designs may offer little to no emission reduction benefit in the 2021 SOT case. However, it is anticipated that it will improve substantially moving to future 2030 performance targets such as higher fuel and co-product yields without increasing the process energy and chemical demands.

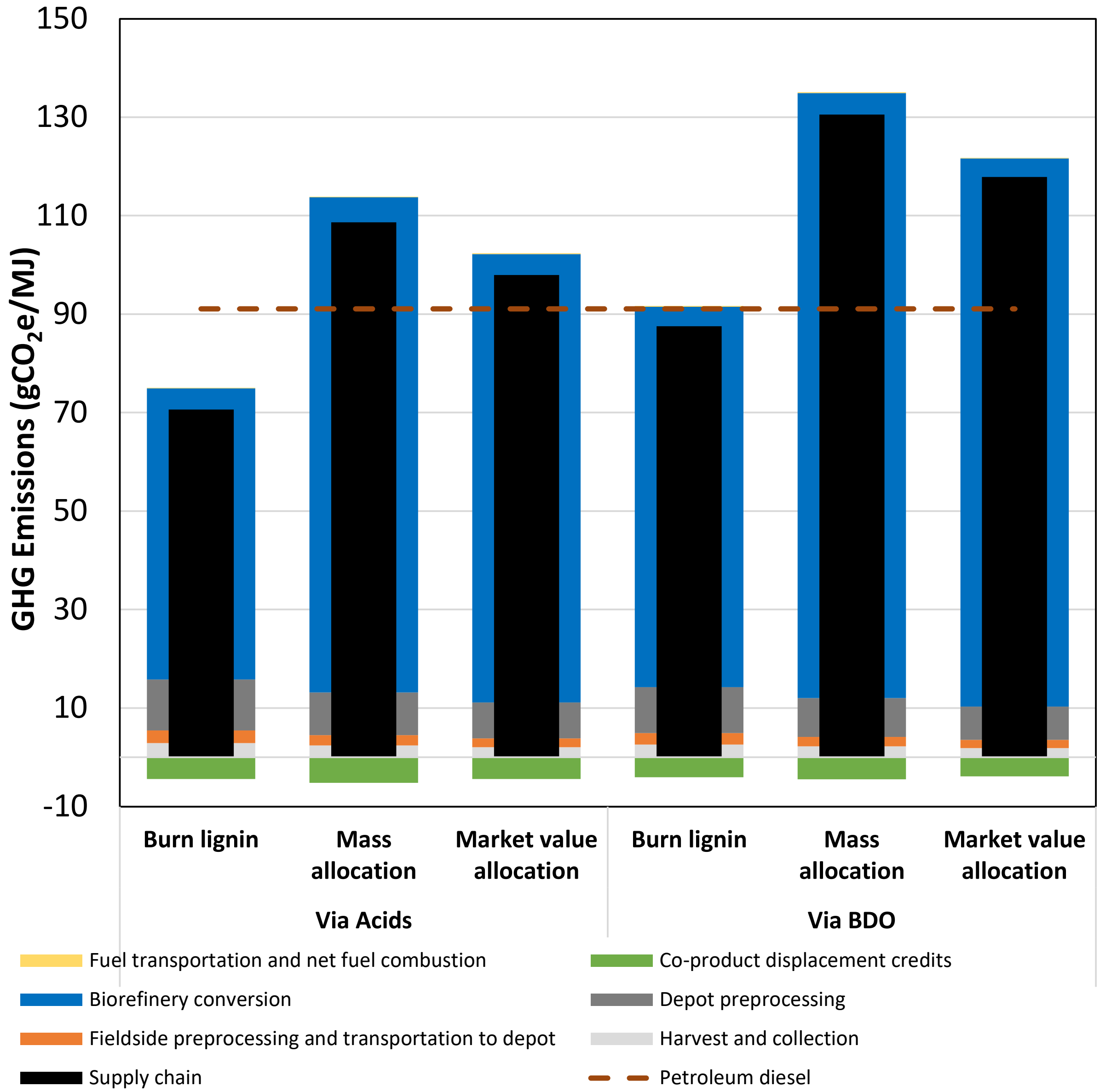


Figure 17 Supply Chain GHG Emissions of Renewable Diesel via Biochemical Conversion, Using the Process-Level Allocation Method to Address Effects of BKA Co-Production

Under the displacement method, all the chemical use and associated emissions are attributed to the hydrocarbon fuels. Meanwhile, the renewable diesel fuels also get all the credits from the lignin-derived BKA co-product displacing conventional fossil-based AA (as both BKA and AA are intended for the same end-product market). In addition, bio-based BKA generates GHG emission credits by sequestering biogenic carbon given that its carbon is derived from herbaceous biomass. BKA production generates -50 to -57 g CO_2e/MJ GHG emission credits from both displacing conventional AA (-44 to -50 g CO_2e/MJ) and biogenic carbon sequestration (-7 to -8 g CO_2e/MJ). As a result, supply chain GHG emission intensities of renewable diesel are

87 and 112 g CO_2e/MJ in the acids and BDO intermediate pathways, respectively, as shown in Figure 18.

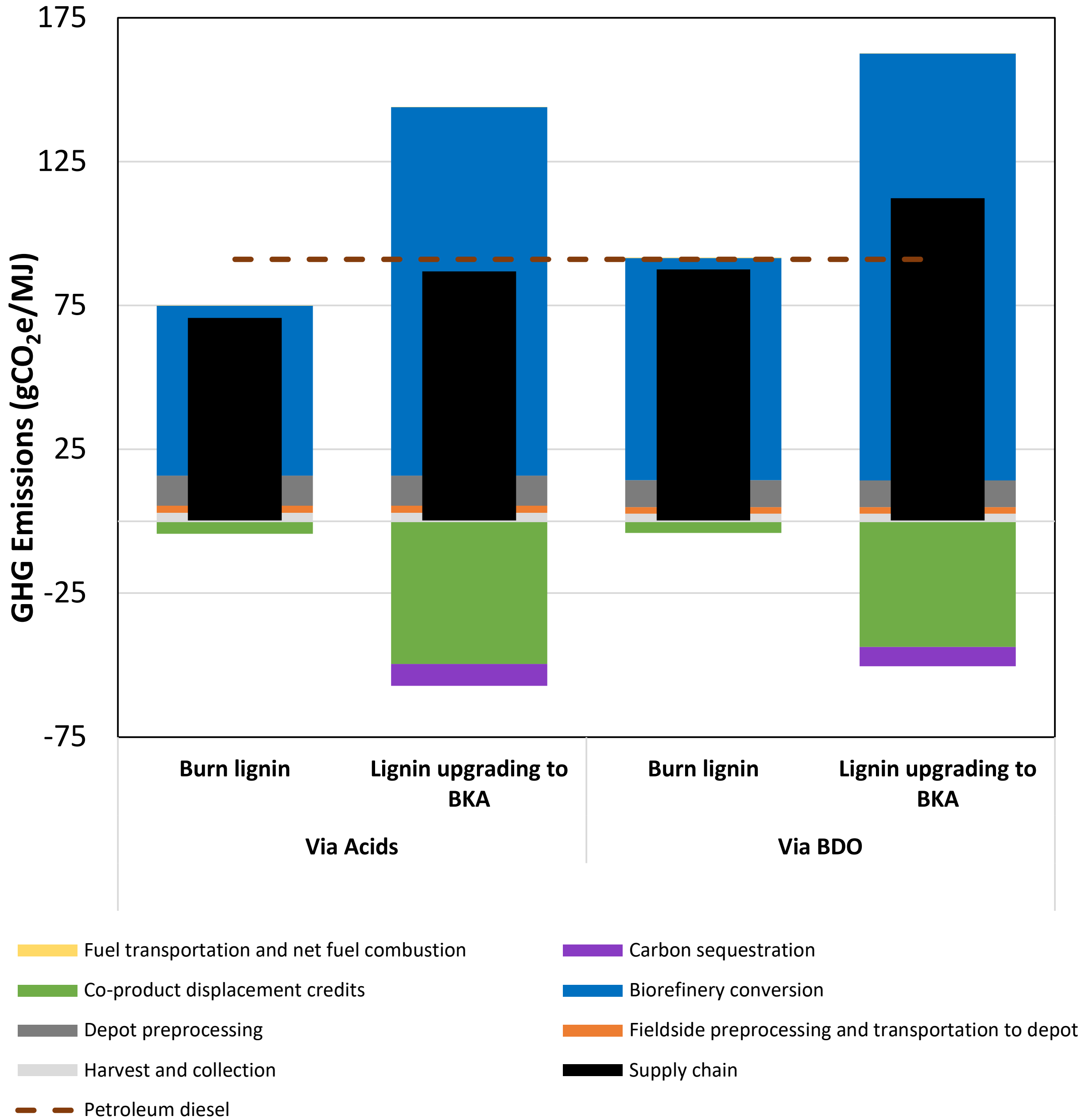
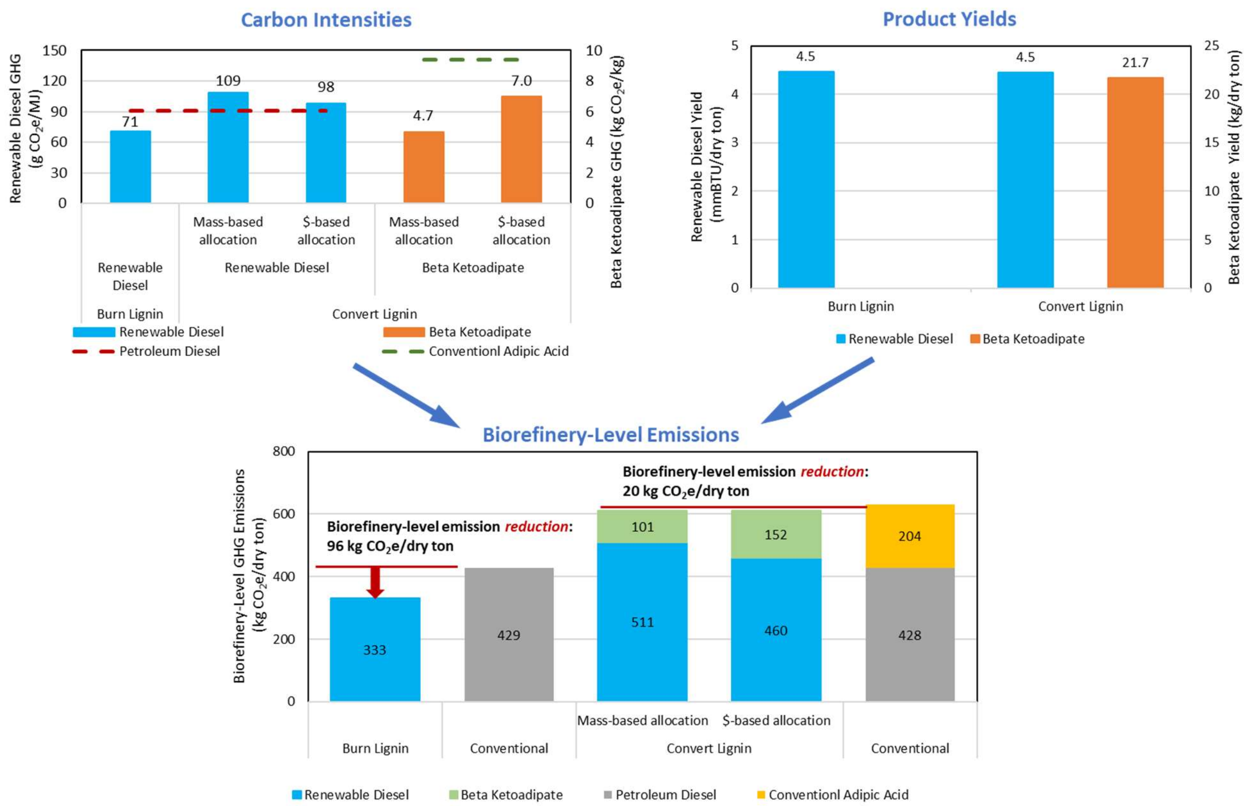


Figure 18 Supply Chain GHG Emissions of Renewable Diesel via Biochemical Conversion, Using the Displacement Method to Address Effects of BKA Co-Production

The biorefinery-level emissions of the biochemical conversion pathway vary among process designs, given variation in yields of the fuels and BKA co-product and in total biorefinery emissions. The burning lignin design in the 2021 SOT case achieved about 96 and 18 kg CO_2e of GHG emission reduction per dry ton of herbaceous feedstock blend converted to renewable diesel with the via acids and BDO intermediate route, respectively, owing to the somewhat lower carbon intensity of renewable diesel fuel compared to that of petroleum diesel.

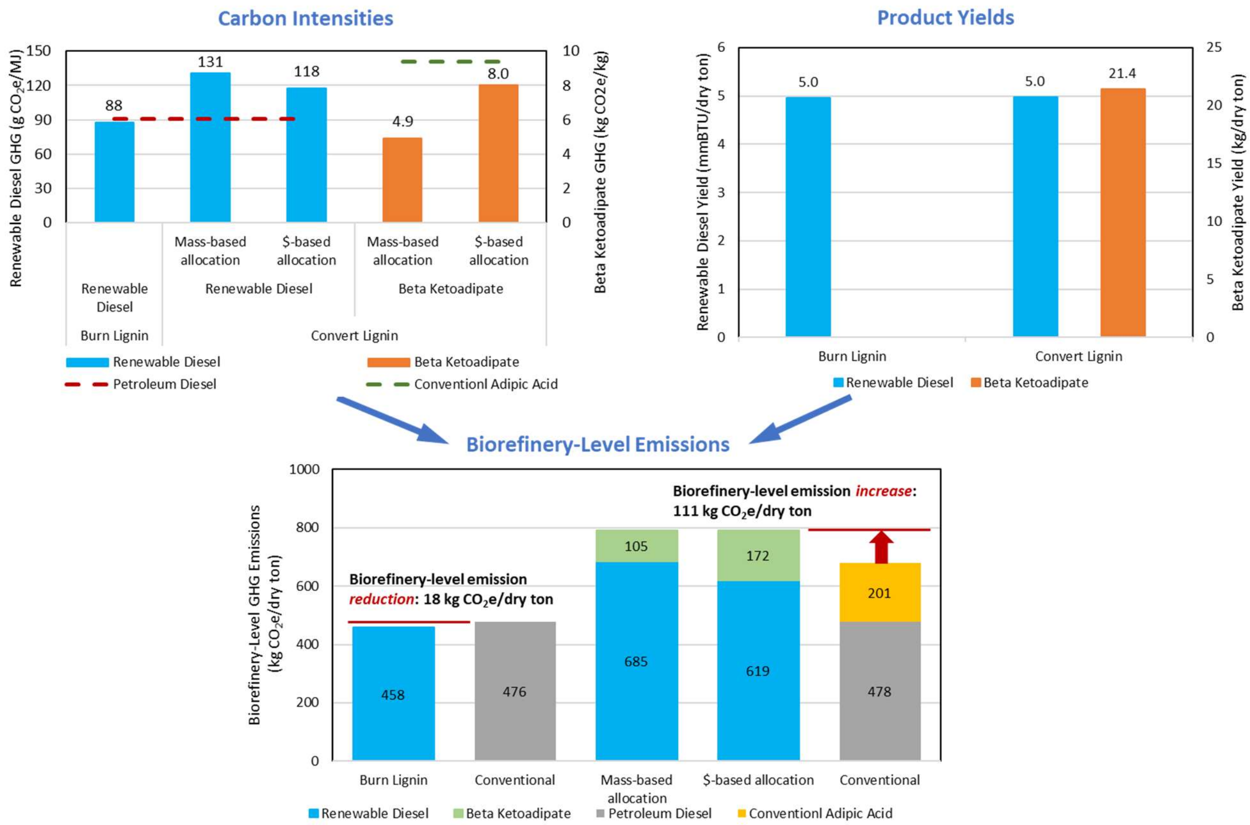
When lignin is converted to the BKA co-product in the 2021 SOT case, we estimated a reduction in biorefinery-level GHG emissions by about 20 kg CO_2e per dry ton of the feedstock blend converted to fuels and BKA for the via acids intermediate route, and an increase in biorefinery-level GHG emissions by about 111 kg CO_2e per dry ton of the feedstock blend converted to fuels and BKA for the via BDO intermediate route (Figure 19).



(a) Via acids

Figure 19 Biorefinery-Level Greenhouse Gas Emissions and Reductions, for the 2021 SOT Case of the Biochemical Conversion Pathway for (a) Via Acids and (b) Via BDO Intermediate Routes

Figure 19 (Cont.)



(b) Via BDO

3.3.2 Supply Chain Water Consumption

Figure 20 shows that the 2021 SOT case has much higher water consumption than that of petroleum diesel. This higher consumption exists regardless of the lignin utilization strategies, intermediate conversion routes, and co-product handling methods, owing to significant embedded water consumption associated with the process chemical use as well as the makeup water requirements during the biochemical conversion process. The embedded water consumption is driven by cooling demands in the process and by process water requirements and losses attributable to biochemical processing at 20 to 30% (by mass) solids with high water flows throughout the conversion process.

Under the purpose-driven, process-level allocation method, total water consumption at the biorefinery conversion step when embedded water for process chemicals is excluded is 14-16 gal/GGE and 7-9 gal/GGE for the acids and BDO routes, respectively, depending on the basis for allocation in the 2021 SOT case. When embedded water for process chemicals is also included, total water consumption at the biorefinery conversion step is 39-43 gal/GGE and 26-28 gal/GGE for the acids and BDO routes, respectively, depending on the basis for allocation.

The acids design uses more water than the BDO design because it uses more makeup water and more chemicals with high embedded water consumption, such as corn steep liquor.

Under the displacement method, water consumption is driven by the conversion process (Figure 21). When lignin is upgarded to BKA via acids, water consumption by the conversion process is 51 gal/GGE. When lignin is upgraded to BKA via BDO, water consumption by the conversion process is 33 gal/GGE.

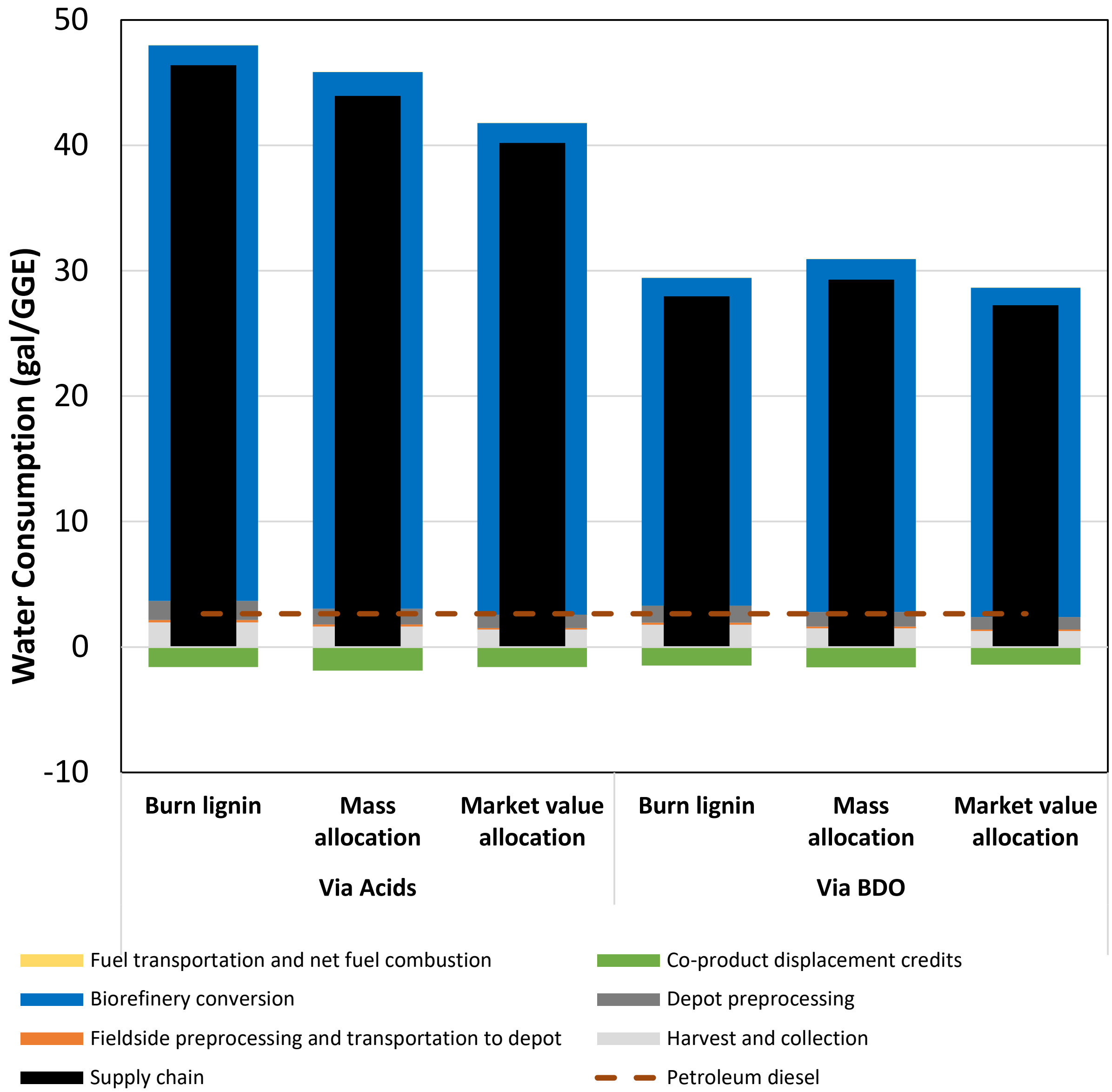


Figure 20 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via Biochemical Conversion, Using the Process-Level Allocation Method to Address Effects of BKA Co-Production, Compared to 2.7 gal/GGE for Petroleum Diesel

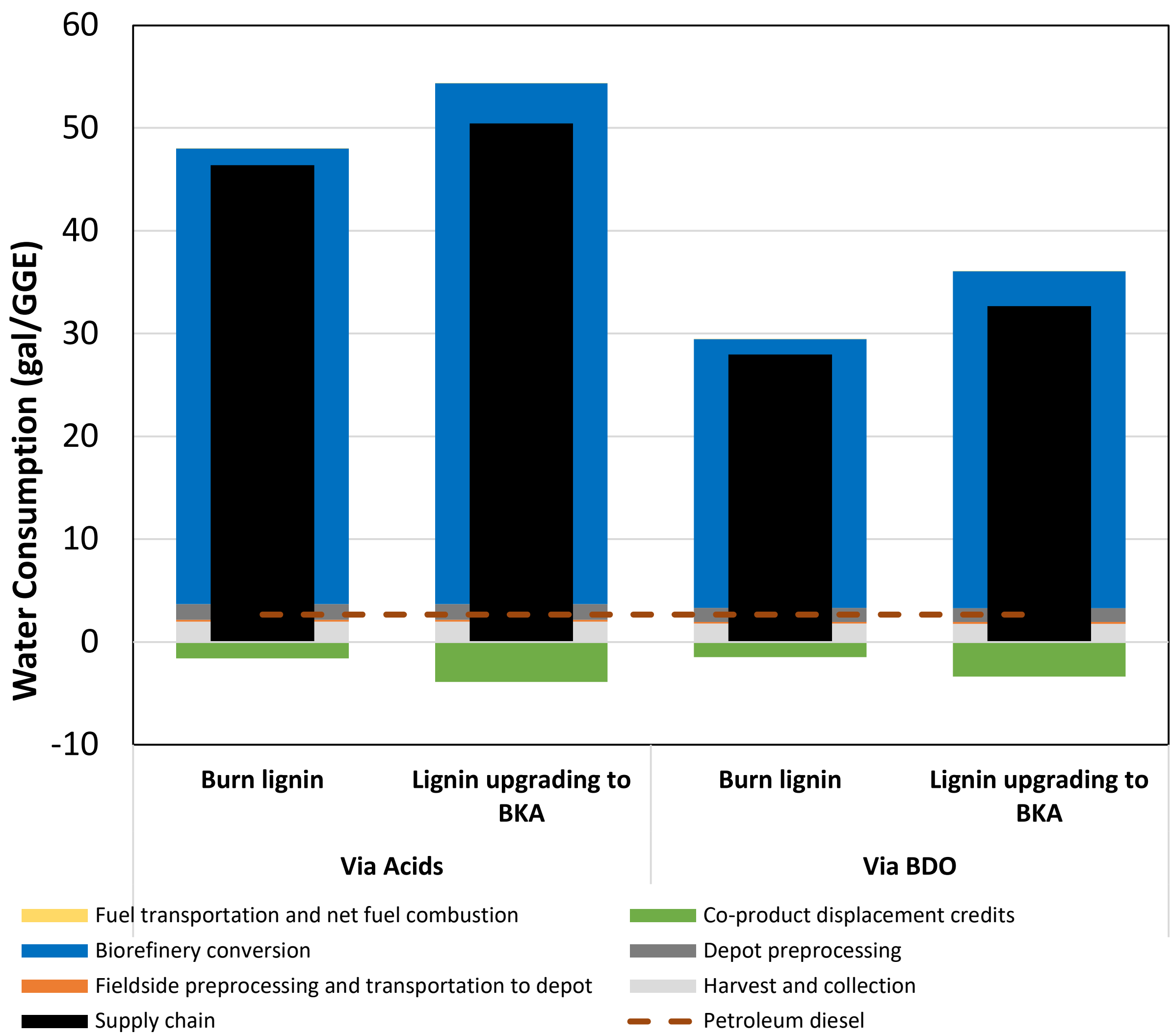


Figure 21 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via Biochemical Conversion, Using the Displacement Method to Address Effects of BKA Co-Production

The direct water consumption during the conversion process increases from 17.9 gal/GGE in the 2020 SOT case to 19.7 gal/GGE in the 2021 SOT case for the via acids pathway, which is a 10% increase in direct water consumption, and increases from 7.8 gal/GGE in the 2020 SOT case to 10.1 gal/GGE in the 2021 SOT case for the via BDO pathway, which is a 29% increase in direct water consumption.

We summarized the biorefinery-level results for water consumption in Table 14 for the biochemical conversion pathway.

3.3.3 Supply Chain NO_x Emissions

Under the process-level allocation method, Figure 22 shows that total NO_x emissions are higher than those of petroleum diesel in the 2021 SOT case regardless of the intermediate pathway and the basis for process-level allocation. Biorefinery conversion is the largest contributor to the NO_x emissions, followed by fuel combustion by vehicles, energy consumption during preprocessing, and harvest/collection of feedstocks using diesel-driven equipment such as harvesters and tractors.

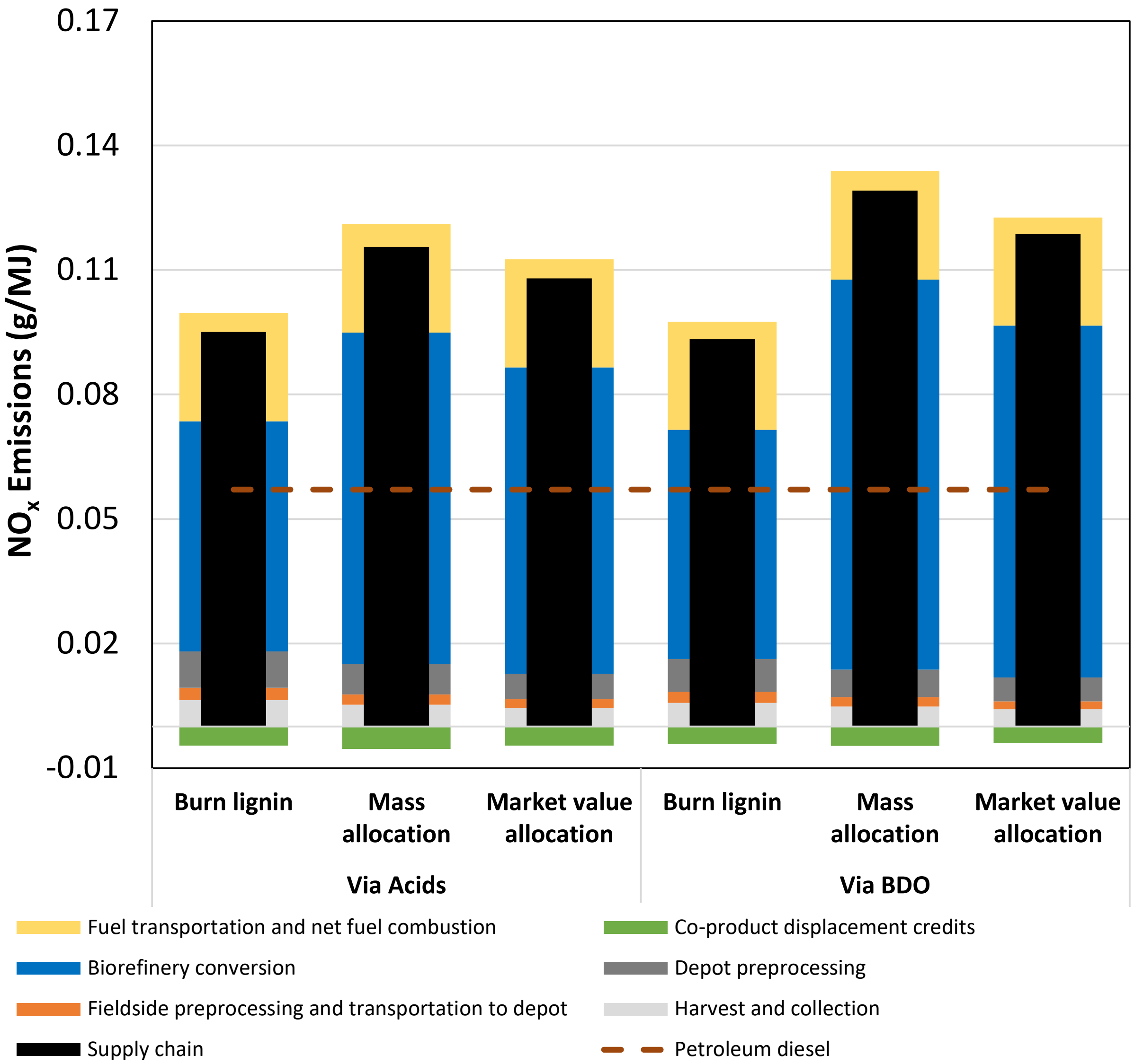


Figure 22 Supply Chain NO_x Emissions (g/MJ) of Renewable Diesel via Biochemical Conversion Using the Process-Level Allocation Method, Relative to 0.06 g/MJ for Petroleum Diesel

Under the displacement method, in the 2021 SOT case the biochemical pathways have higher NO_x emissions than petroleum diesel when lignin is burned for energy, but lower NO_x emissions when lignin is upgraded to BKA (Figure 23).

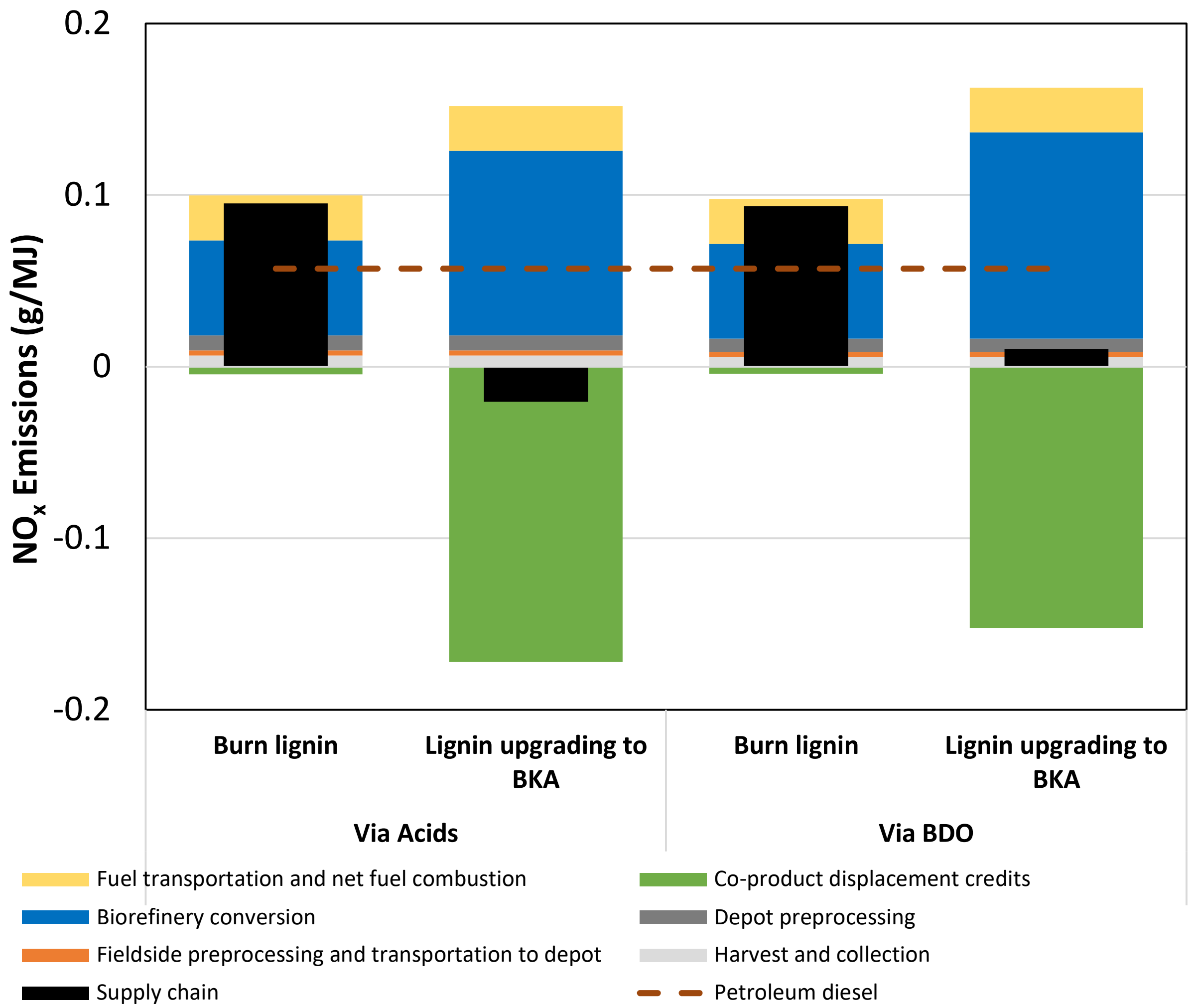


Figure 23 Supply Chain NOx Emissions (g/MJ) of Renewable Diesel via Biochemical Conversion, Using the Displacement Method to Address Effects of BKA

3.3.4 Summary of Sustainability Metrics

Tables 11 summarizes supply chain sustainability metrics, including fossil energy consumption, NEB, GHG emissions, water consumption, and NO_x emissions of renewable diesel from these biochemical conversion designs, using the process-level allocation method. GHG emissions estimated by market-value-based allocation are lower than those estimated by mass-based allocation because renewable diesel has a lower market value than the BKA product on a per-kg basis. Thus, a smaller portion of the emission burdens are allocated to renewable diesel by market value than by mass.

Table 11 Supply Chain Sustainability Metrics for Renewable Diesel via Biochemical Pathway, 2021 SOT Case

	Scenario 1: Via Acids			Scenario 2: Via BDO			
		Lignin upgrading to beta ketoadipate			Lignin upgrading to beta ketoadipate		
	Burning lignin	Mass-based allocation	Market-value-based allocation	Burning lignin	Mass-based allocation	Market-value-based allocation	Petroleum Diesel
			Biofuel yield				
mmBtu/dry ton	4.5	5.4	6.3	5.0	5.9	6.8	
			Co-product yield				
Sodium sulfate, Kg/mmBtu of biofuel	25.1	29.7	25.1	23.2	25.6	22.0	
			Fossil energy consumption				
MJ/MJ	0.9	1.4	1.3	1.2	1.8	1.7	1.2
			Net energy balance				
MJ/MJ	0.1	-0.4	-0.3	-0.2	-0.8	-0.7	
			GHG emissions[a]				
g CO_2e/MJ	71 (-22%)	109 (19%)	98 (8%)	88 (-4%)	131 (43%)	118 (29%)	91
g CO_2e/ GGE	8,649	13,305	11,994	10,725	15,990	14,438	11,157
			Water consumption				
L/MJ	1.4	1.4	1.2	0.9	0.9	0.8	0.1
gal/GGE	46.4	43.9	40.2	28.0	29.3	27.3	2.7
			Total NO_x emissions				
g NO_x/MJ	0.10	0.12	0.11	0.09	0.13	0.12	0.06
g NO_x/GGE	11.6	14.2	13.2	11.4	15.8	14.5	7.0
			Urban NO_x emissions				
g NO_x/MJ	0.02	0.03	0.03	0.03	0.03	0.03	0.03
g NO_x/GGE	3.0	3.9	3.7	3.3	3.6	3.5	3.3

[a] The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

Tables 12 summarizes the supply chain sustainability metrics of BKA, which displaces conventional AA that are mainly used to produce nylon, produced from the acid and BDO pathways in 2021 SOT case under the purpose-driven, process-level allocation method. Under this method, lignin-derived BKA could achieve reductions in GHG emissions by about 48%-50% (mass-based allocation) and 15%-26% (market value-based allocation), relative to conventional natural gas (NG)-based AA in the 2021 SOT case.

Table 12 Supply Chain Sustainability Metrics for Beta Ketoadipate via Biochemical Pathway, 2021 SOT Case

	Scenario 1: Via Acids		Scenario 2: Via BDO		
	Mass-based allocation	Market-value-based allocation	Mass-based allocation	Market-value-based allocation	Conventional AA
			BKA yield		
ton/dry ton	0.14	0.080	0.15	0.087	
			Fossil energy consumption		
MJ/kg	85.0	115.1	92.1	136.0	104.6
			GHG emissions[a]		
g CO_2e/kg	4,673 (-50%)	6,994 (-26%)	4,916 (-48%)	8,019 (-15%)	9,397
			Water consumption		
L/kg	54.5	79.6	36.5	52.0	11.0
			Total NO_x emissions		
g NO_x/kg	6.4	8.1	6.8	9.4	35.9

[a] The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

Table 13 summarizes the supply chain sustainability metrics, including fossil energy consumption, NEB, GHG emissions, water consumption, and NO_x emissions of renewable diesel from these biochemical conversion designs, using the displacement method.

Table 13 Supply Chain Sustainability Metrics for Renewable Diesel via Biochemical Pathway in the 2021 SOT Case, Using the Displacement Method

	Scenario 1: Via Acids		Scenario 2: Via BDO		
	Burning lignin	Lignin upgrading to BKA	Burning lignin	Lignin upgrading to BKA	Petroleum Diesel
			Biofuel yield		
mmBtu/dry ton	4.5	4.5	5.0	5.0	
			Co-product yield		
BKA, kg/mmBtu of biofuel	0	4.9	0	4.3	
Sodium sulfate, kg/mmBtu of biofuel	25.1	35.8	23.2	30.2	
			Fossil energy consumption		
MJ/MJ	0.9	1.3	1.2	1.8	1.2
			Net energy balance		
MJ/MJ	0.1	-0.3	-0.2	-0.8	
			GHG emissions		
g CO_2e/MJ	71 (-22%)	87 (-5%)	88 (-4%)	112 (23%)	91
g CO_2e/ GGE	8,649	10,637	10,725	13,749	11,157
			Water consumption		
L/MJ	1.4	1.6	0.9	1.0	0.1
gal/GGE	46.4	50.4	28.0	32.7	2.7
			Total NO_x emissions		
g NO_x/MJ	0.10	-0.02	0.09	0.01	0.06
g NO_x/GGE	11.6	-2.5	11.4	1.3	7.0
			Urban NO_x emissions		
g NO_x/MJ	0.02	0.03	0.03	0.03	0.03
g NO_x/GGE	3.0	4.1	3.3	3.8	3.3

Tables 14 summarizes biorefinery-level sustainability metrics for the biochemical pathway. For fossil energy consumption, GHG emissions, water consumption, and NO_x emissions, we present supply chain direct impacts per ton of biomass converted to both RD and BKA co-product, the total displacement credit from RD, the total displacement credit from lignin-derived BKA, and the net, combined impacts from both RD and BKA.

Table 14 Biorefinery-Level Sustainability Metrics of the Biochemical Pathway, 2021 SOT Case

	Scenario 1: Via Acids			Scenario 2: Via BDO			
		Lignin upgrading to BKA			Lignin upgrading to BKA		
	Burn lignin	Mass-based allocation	Market-value-based allocation	Burn lignin	Mass-based allocation	Market-value-based allocation	
Products							
Renewable diesel	4.5	4.5		5.0	5.0		mmBtu/dry ton biomass
BKA	-	0.02		-	0.02		ton/dry ton biomass
Fossil energy consumption							
Direct consumption by RD production	4,197	6,606	5,954	6,066	9,672	8,730	MJ/dry ton biomass
Credits from RD production	-5,651	-5,641	-5,641	-6,277	-6,296	-6,296	MJ/dry ton biomass
Net consumption by RD production	*-1,454*	*966 (178%)*	*313 (58%)*	*-210*	*3,376 (109%)*	*2,434 (78%)*	MJ/dry ton biomass
Direct consumption by BKA production	-	1,843	2,496	-	1,973	2,914	MJ/dry ton biomass
Credits from BKA production	-	-2,267	-2,267	-	-2,240	-2,240	MJ/dry ton biomass
Net consumption by BKA production	-	*-424 (-78%)*	*229 (42%)*	-	*-267 (-9%)*	*674 (22%)*	MJ/dry ton biomass
Net total consumption	-1,454	542		-210	3,108		MJ/dry ton biomass
GHG emissions							
Direct emissions from RD production	333	511	460	458	685	619	kg/dry ton biomass
Credits from RD production	-429	-428	-428	-476	-478	-478	kg/dry ton biomass
Net emissions from RD production	*-96*	*82 (-413%)*	*32 (-161%)*	*-18*	*207 (186%)*	*141 (127%)*	kg/dry ton biomass
Direct emissions from BKA production	-	101	152	-	105	172	kg/dry ton biomass
Credits from BKA production	-	-204	-204	-	-201	-201	kg/dry ton biomass

Table 14 (Cont.)

	Scenario 1: Via Acids			Scenario 2: Via BDO			
		Lignin upgrading to BKA			Lignin upgrading to BKA		
	Burn lignin	Mass-based allocation	Market-value-based allocation	Burn lignin	Mass-based allocation	Market-value-based allocation	
Net emissions from BKA production	-	*-102 (513%)*	*-52 (261%)*	-	*-96 (-86%)*	*-30 (-27%)*	kg/dry ton biomass
Net total emissions	-96	-20		-18	111		kg/dry ton biomass
Water consumption							
Direct consumption by RD production	1,784	1,687	1,542	1,194	1,255	1,167	gal/dry ton biomass
Credits from RD production	-102	-102	-102	-114	-114	-114	gal/dry ton biomass
Net consumption by RD production	*1,681*	*1,584 (86%)*	*1,440 (79%)*	*1,080*	*1,141 (89%)*	*1,053 (82%)*	gal/dry ton biomass
Direct consumption by BKA production	-	312	456	-	207	294	gal/dry ton biomass
Credits from BKA production	-	-63	-63	-	-62	-62	gal/dry ton biomass
Net consumption by BKA production	-	*249 (14%)*	*393 (21%)*	-	*145 (11%)*	*232 (18%)*	gal/dry ton biomass
Net total consumption	1,681	1,834		1,080	1,285		gal/dry ton biomass
Total NO_x emissions							
Direct emissions from RD production	447	543	508	488	677	622	g/dry ton biomass
Credits from RD production	-269	-268	-268	-299	-300	-300	g/dry ton biomass
Net emissions from RD production	*178*	*275 (-75%)*	*239 (-66%)*	*189*	*378 (-154%)*	*323 (-131%)*	g/dry ton biomass
Direct emissions from BKA production	-	139	175	-	147	201	g/dry ton biomass
Credits from BKA production	-	-779	-779	-	-770	-770	g/dry ton biomass
Net emissions from BKA production	-	*-640 (175%)*	*-604 (166%)*	-	*-623 (254%)*	*-568 (231%)*	g/dry ton biomass
Net total emissions	178	-365		189	-245		g/dry ton biomass

Note: Positive net totals indicate net increases compared to conventional products. Negative net totals indicate net reductions compared to conventional products. The values in parentheses are contributions to the net totals by RD and co-product in percentage.

3.4 Algae Hydrothermal Liquefaction

3.4.1 Supply Chain Greenhouse Gas Emissions

Figure 24 shows the supply chain GHG emissions and their key contributing supply chain processes, in g CO_2e/MJ, of RD in the 2021 compared to a life-cycle carbon intensity of 91 g CO_2e/MJ for petroleum diesel. RD reduces GHG emissions by 107%. The HTL conversion processes, which consume grid electricity, natural gas for hydrogen production, and chemicals and catalysts for biocrude production and upgrading, contribute to about 21.0 g CO_2e/MJ. Waste-derived algae does not require external nutrients such as nitrogen or phosphorus and does not require dedicated CO_2 sourcing and transportation, which could otherwise be energy- and emission-intensive. Algae dewatering via centrifuge and transportation of algae to the HTL biorefinery contribute 3.3 g CO_2e/MJ. The hydrogen production via steam methane reforming of natural gas is responsible for about 11.0 g CO_2e/MJ. The struvite co-product recovered from the aqueous HTL wastewater generates a credit of -31 g CO_2e/MJ by displacing synthetic nitrogen and phosphorous fertilizers.

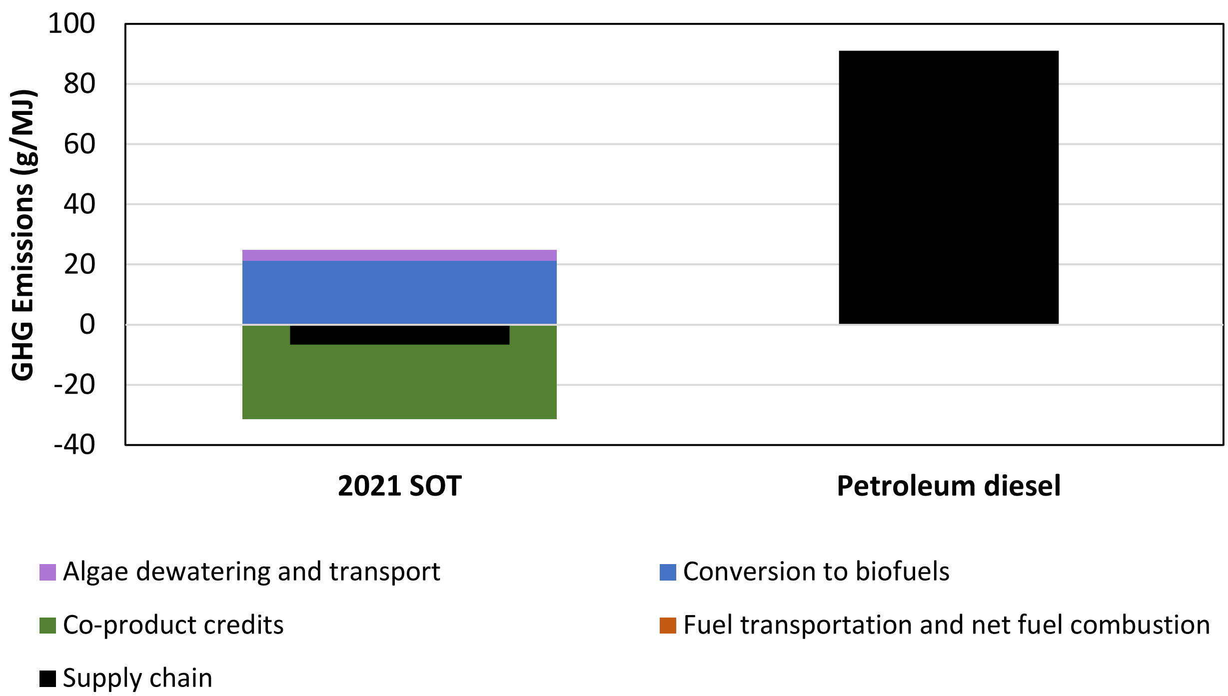


Figure 24 Supply Chain GHG Emissions (g CO_2e/MJ) of Renewable Diesel via Waste-Derived Algae HTL

A biorefinery-level GHG emission reduction could be expected for the WWTP algae HTL pathway (Figure 25). An emission reduction of about 878 kg CO_2e per dry ton of algae converted to fuels can be achieved in the 2021 SOT case.

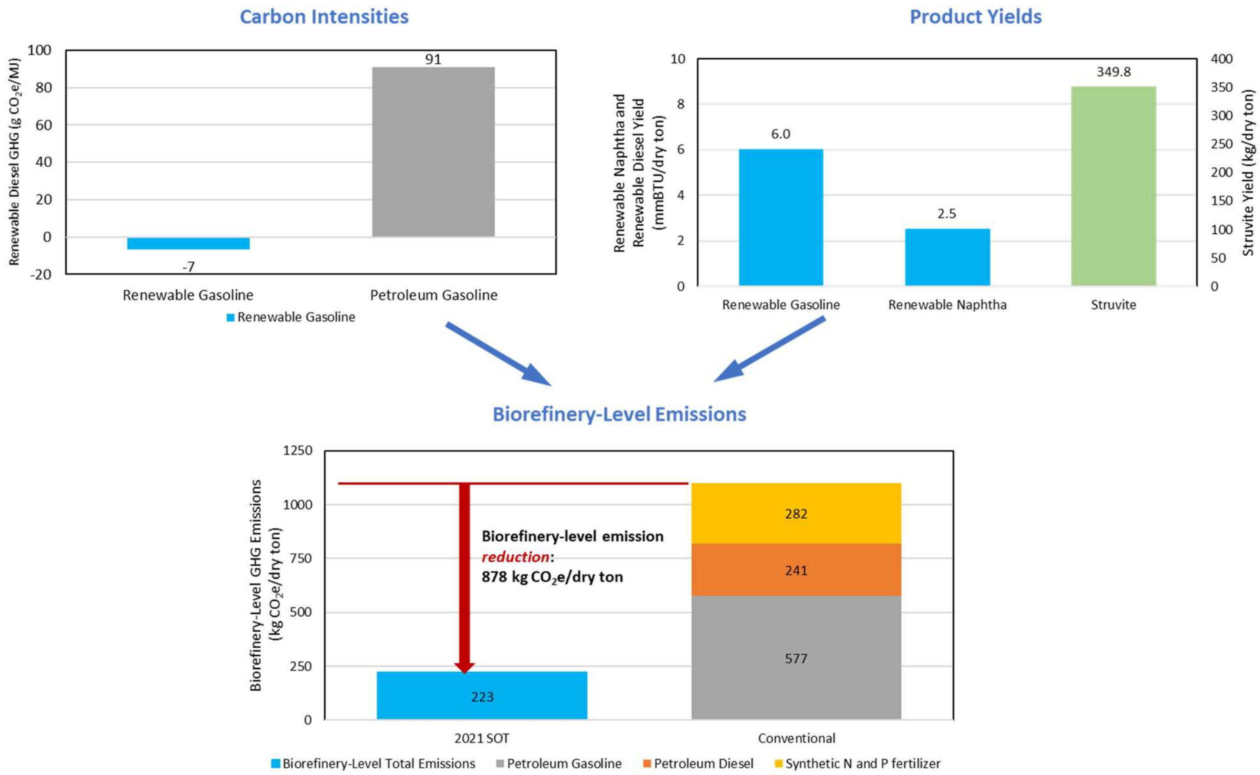


Figure 25 Biorefinery-Level Greenhouse Gas Emissions and Reductions, the 2021 SOT Case of the Waste-Derived Algae HTL Pathway

3.4.2 Supply Chain Water Consumption

In the 2021 SOT case, water consumption associated with natural gas consumption for hydrogen production and with chemical and catalyst use during the HTL processes is the major contributor to supply chain water consumption (Figure 26). Overall, the 2021 SOT case has negative supply chain water consumption due to the credit of the struvite co-product displacing synthetic nitrogen and phosphorous fertilizers.

The direct water consumption during the conversion process increases substantially from 0.8 gal/GGE in the 2020 SOT case to 7.5 gal/GGE due to the overhaul of the design of the conversion process, which is an 838% increase in direct water consumption.

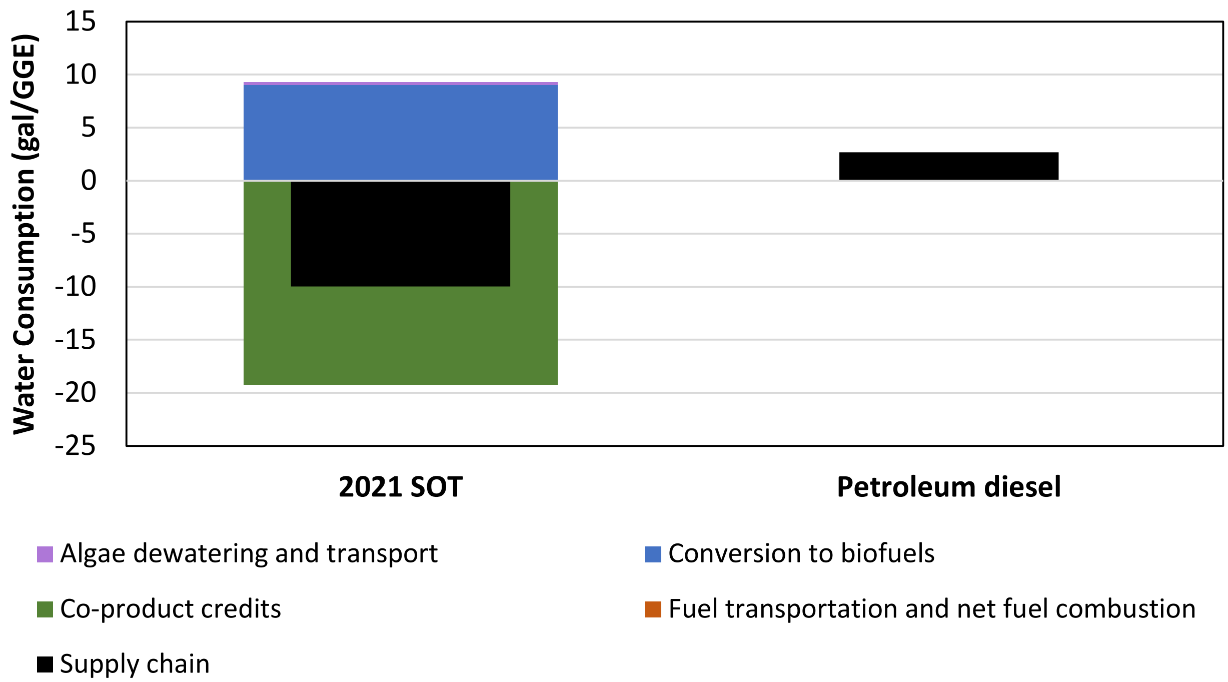


Figure 26 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via Waste-Derived Algae HTL, Compared to 2.7 gal/GGE for Petroleum Diesel

3.4.3 Supply Chain NO_x Emissions

The total NO_x emissions are about 162% lower than those of petroleum diesel in the 2021 SOT. The negative supply chain NO_x emissions are mainly due to the credit of the struvite co-product displacing synthetic nitrogen and phosphorous fertilizers.

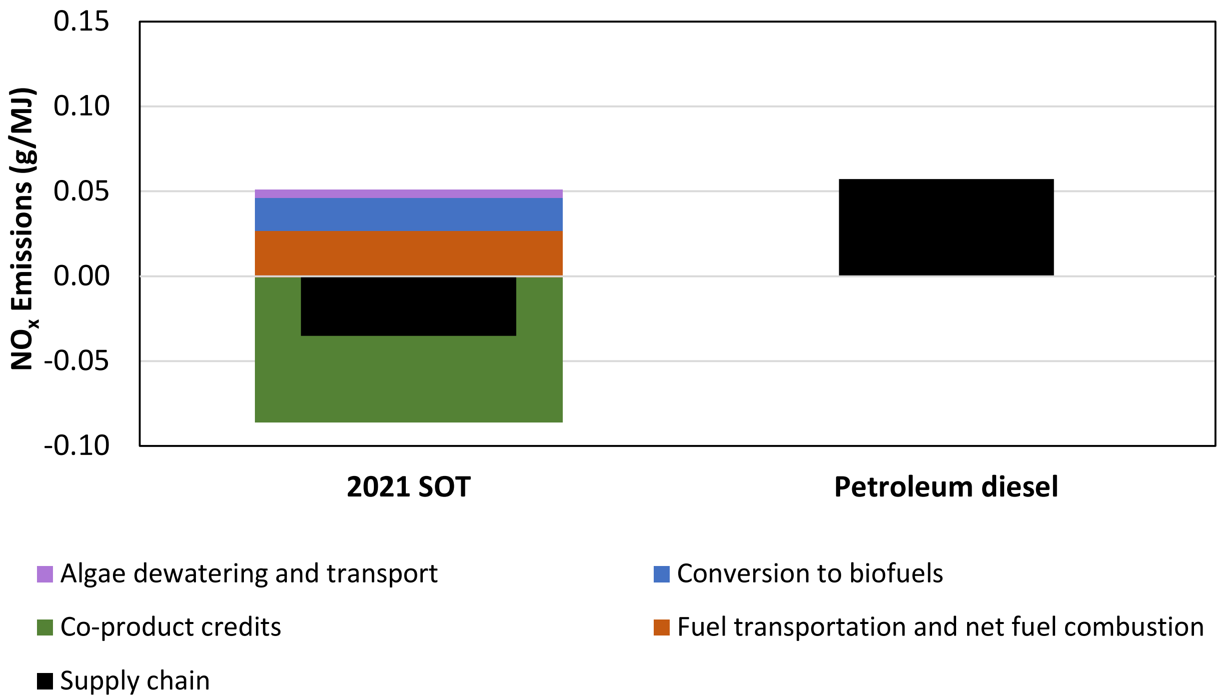


Figure 27 Supply Chain NO_x Emissions (g/MJ) of Renewable Diesel via Waste-Derived Algae HTL, Compared to 0.06 g/MJ for Petroleum Diesel

3.4.4 Summary of Sustainability Metrics

Table 15 summarizes the supply chain sustainability metrics, including fossil energy consumption, NEB, GHG emissions, water consumption, and NO_x emissions of renewable diesel from the WWTP algae HTL pathway.

Table 15 Supply Chain Sustainability Metrics for Renewable Diesel via Algae/Corn Stover Pathway in the 2021 SOT Case, Using the Displacement Method

	2021 SOT		Petroleum Diesel
		Biofuel yield	
mmBtu/dry ton	8.5		
		Fossil energy consumption	
MJ/MJ	-0.1 (-109%)		1.2
		Net energy balance	
MJ/MJ	1.1		
		GHG emissions	
g CO_2e/MJ	-6.6 (-107%)		91
g CO_2e/ GGE	-810		11,157
		Water consumption	
L/MJ	-0.31		0.08
gal/GGE	-10.0		2.7
		Total NO_x emissions	
g NO_x/MJ	-0.04		0.06
g NO_x/GGE	-4.3		7.0
		Urban NO_x emissions	
g NO_x/MJ	0.02		0.03
g NO_x/GGE	2.0		3.3

3.5 Combined Algae Processing

The SCSA of the CAP pathway incorporates the 2021 SOT case for algae biomass cultivation with minimally lined ponds using saline algae strains as well as the 2021 SOT case for CAP conversion for both the acids and BDO pathway designs. The purpose-driven, process-level allocation method is applied to address the effect of the PU co-product.

3.5.1 Supply Chain Greenhouse Gas Emissions

Figure 28 shows the supply chain GHG emissions and their key contributing supply chain processes, in g CO_2e/MJ, of RD in the 2021 SOT case, using the mass- and market value-based, process-level allocation method, relative to a life-cycle carbon intensity of 91 g CO_2e/MJ for petroleum diesel. GHG emissions of RD in the 2021 SOT cases are about 35% and 19% lower for the acids and BDO pathways, respectively, than those of petroleum diesel with mass-based process-level allocation. The market value-based process-allocation method suggests reductions in GHG emissions by 62% and 47%, respectively, for the acids and BDO pathways, relative to petroleum diesel.

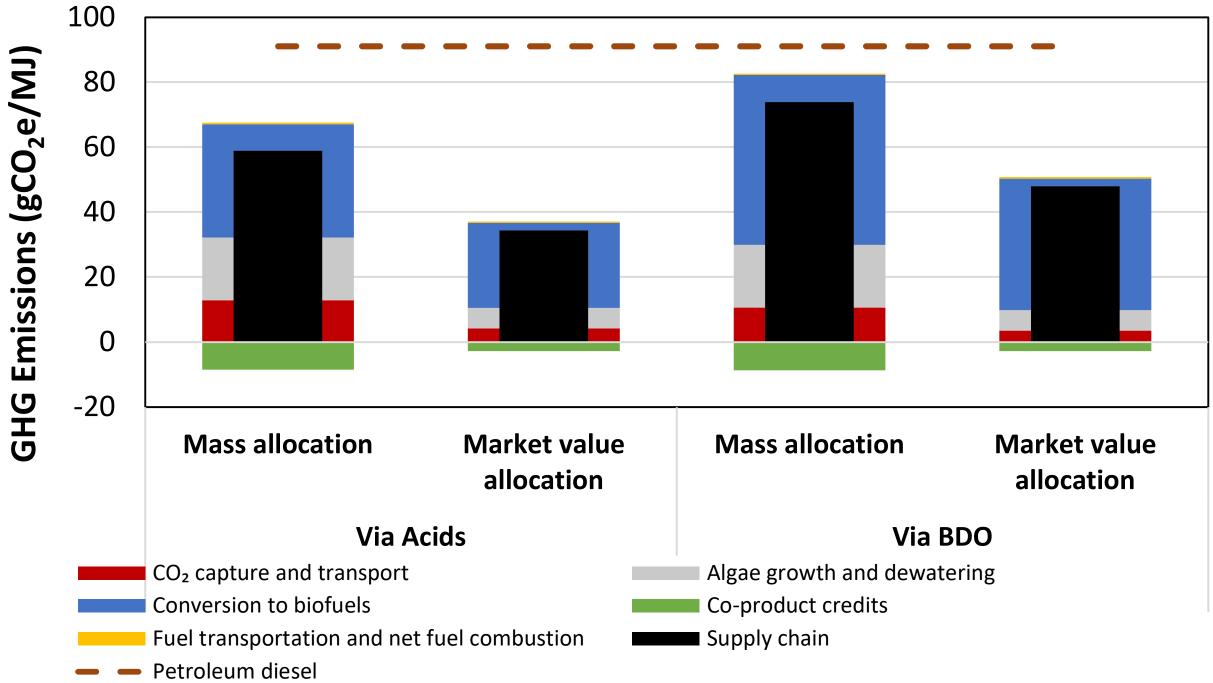


Figure 28 Supply Chain GHG Emissions of Renewable Diesel via CAP Using the Process-Level Allocation Method, Compared to 91 g CO_2e/MJ for Petroleum Diesel

Manufacturing of chemicals and catalysts for use in the CAP conversion processes is the primary emission source in the 2021 SOT case. Energy consumption for algae growth and dewatering and for CO_2 capture and transportation to the algae farm are also notable emission sources. Recycling nutrients from the AD effluent reduces the demand for makeup nutrients for algae cultivation and thus contributes to reducing the emission impacts for the algae production phase. The co-product credits shown in Figure 28 are from surplus electricity displacing U.S. average grid mix. The displacement method is used for surplus electricity because it accounts for only 16% by energy relative to fuel in the 2021 SOT case, which is much smaller than 115%-116% for PU by mass relative to fuel in the 2021 SOT case. The market value-based allocation results lead to lower emissions than those with the mass-based allocation methods because the market value of renewable diesel ($2.5/GGE, or $0.39/lb) is lower than that of PU ($2.04/lb) on a mass basis.

Under the displacement method, all chemical use and associated emissions are attributed to the hydrocarbon fuels. Meanwhile, the hydrocarbon fuels get all the credits from the PU co-product displacing conventional fossil-based PU. In addition, bio-based PU generates GHG emission credits by sequestration of biogenic carbon, given that it contains biogenic carbon derived from algal biomass (the overall carbon content of the PU is 66%, 73% of which is biogenic per process modeling). The production of PU has a significant impact on the GHG emissions in the 2021 SOT case because of a significant PU yield, generating more than -100 g CO_2e/MJ displacement credits by displacing conventional PU (-104 – -105 g CO_2e/MJ) and biogenic carbon sequestration (-47 g CO_2e/MJ). The BDO pathway has higher GHG emissions than the acids pathway because it consumes more hydrogen and natural gas in the conversion process.

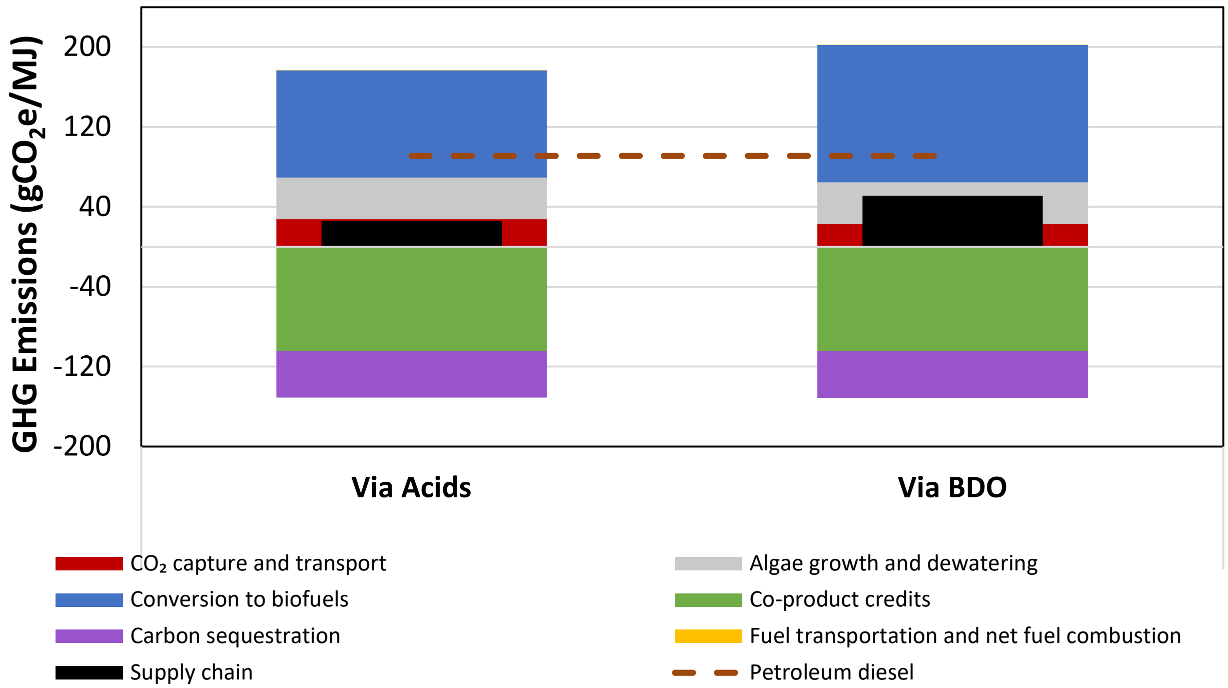
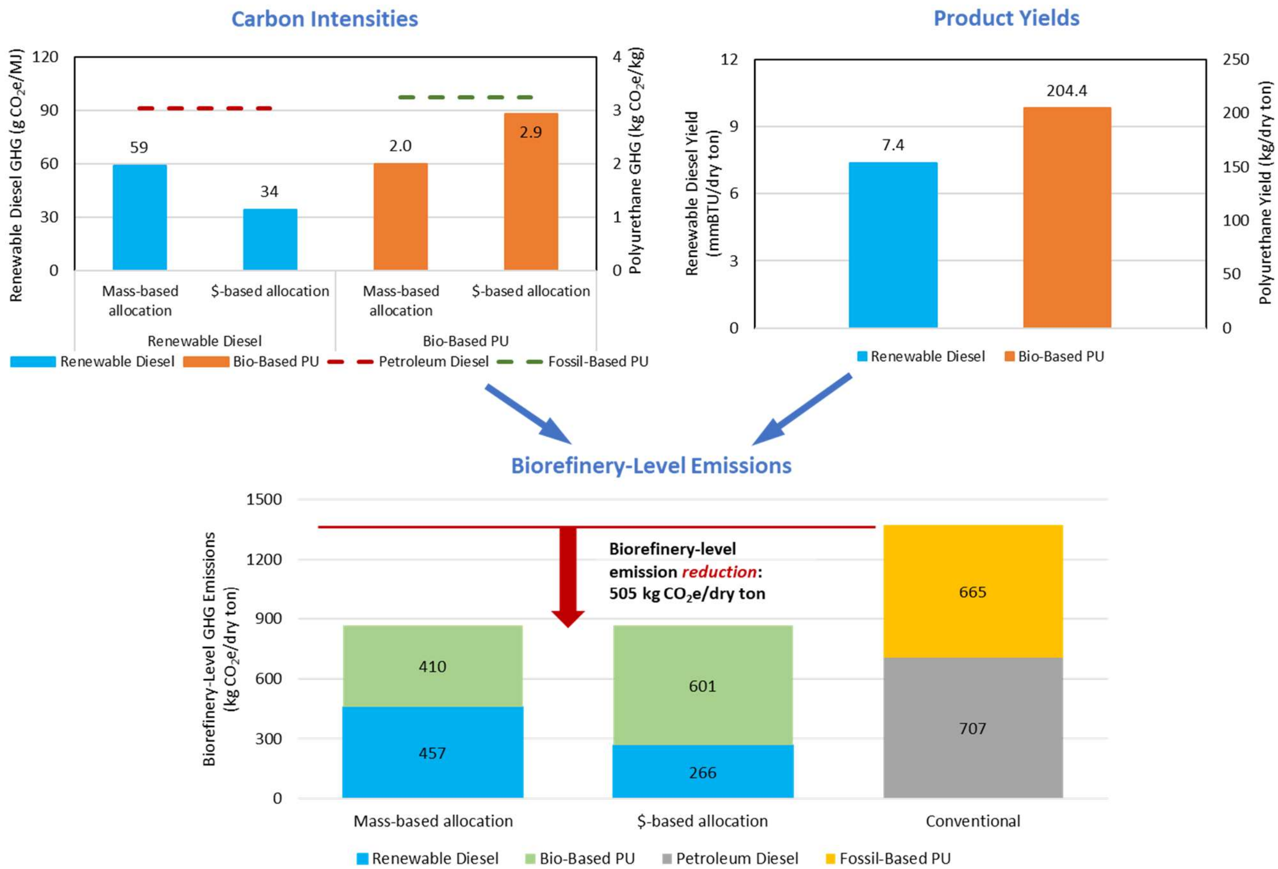


Figure 29 Supply Chain GHG Emissions of Renewable Diesel via CAP, Using the Displacement Method to Address Effects of PU Co-Production

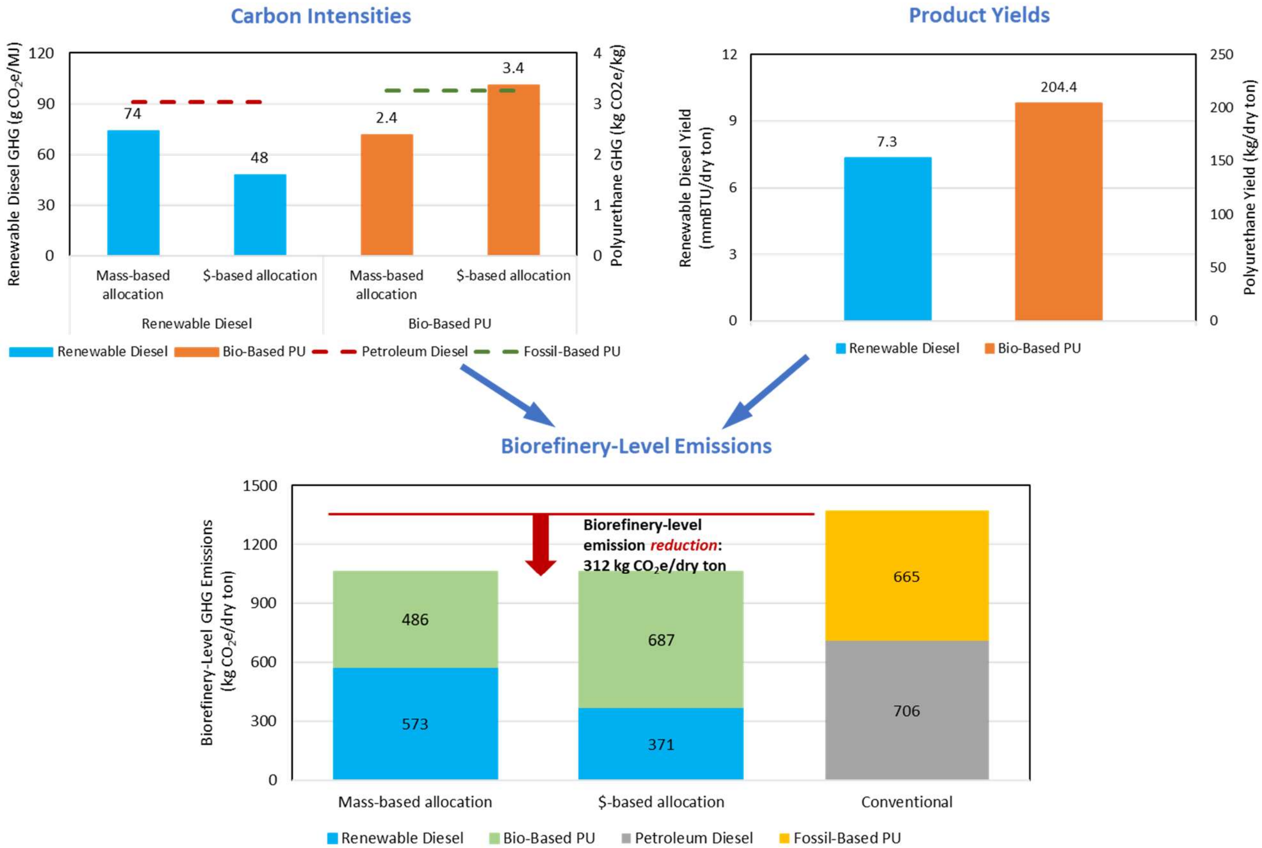
A biorefinery-level GHG emission reduction could be expected for the algae CAP conversion pathway. With the via acids intermediate route, the biorefinery-level emission reduction is about 505 kg CO_2e per dry ton of algae converted to fuels and PU, as shown in Figure 30. With the via BDO intermediate route, the biorefinery-level emission reduction varies from about 312 kg CO_2e per dry ton of algae converted to fuels and PU.



(a) Via acids

Figure 30 Biorefinery-Level Greenhouse Gas Emissions and Reductions, for the 2021 SOT Case of the CAP Conversion Pathway for (a) Via Acids and (b) Via BDO Intermediate Routes

Figure 30 (Cont.)



(b) Via BDO

3.5.2 Supply Chain Water Consumption

Figure 31 shows that the 2021 SOT case has higher water consumption than that of petroleum diesel, owing to significant water consumption associated with the process chemical and catalyst use as well as the makeup water requirements for the CAP conversion process. Direct makeup water consumption within the biorefinery process is 2-5 and 9-13 gal/GGE for the acids and BDO pathways, respectively, depending on the basis (mass or market value) for the process-level allocation (excluding water consumption embedded in chemical usage). Total water consumption within the biorefinery is 24-28 gal/GGE and 14-18 gal/GGE for the acids and BDO pathways, respectively, when water consumption embedded in chemical usage is included. The total water consumption of the acids pathway is high because it uses significantly more corn steep liquor, which is water intensive to make, than the BDO pathway. Water consumption associated with electricity consumption for algae cultivation and dewatering is another major driver. According to algae cultivation models, saline makeup water inputs are required for algae cultivation but do not contribute to freshwater consumption for the CAP pathway.

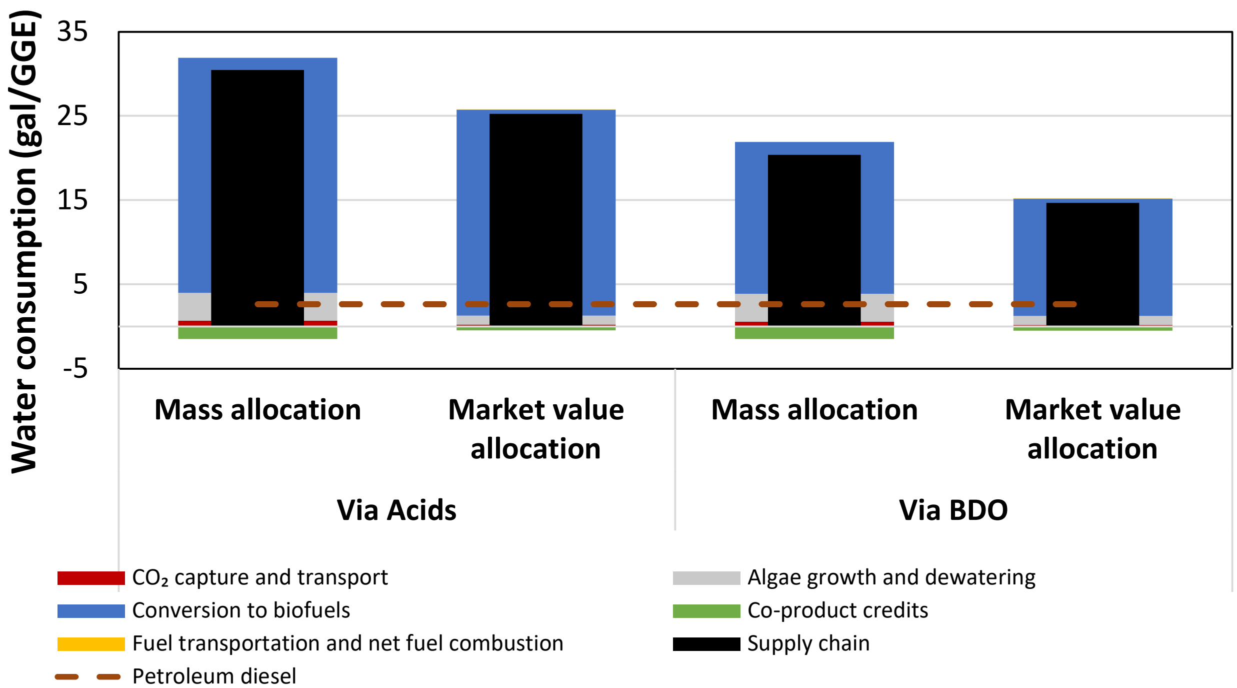


Figure 31 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via CAP Using the Process-Level Allocation Method, Compared to 2.7 gal/GGE for Petroleum Diesel

Under the displacement method, direct makeup water consumption and water consumption associated with chemical use during conversion are the major contributors to supply chain water consumption (Figure 32). Water consumption associated with energy consumption for algae cultivation and dewatering is another major driver of water consumption. Saline water evaporation in the pond or lost in blowdown during cultivation of saline algae strains does not contribute to water consumption because we consider only fresh water consumption in this analysis. The PU co-product generates a displacement credit by displacing conventional fossil-based PU.

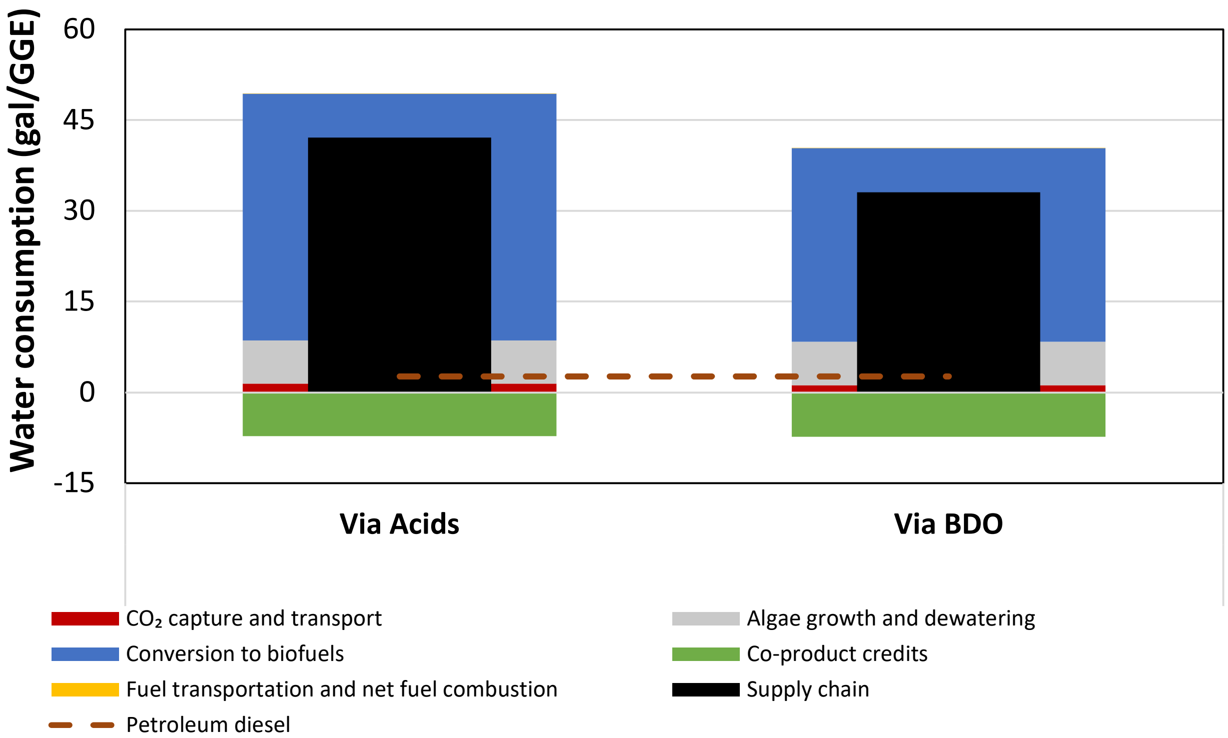


Figure 32 Supply Chain Water Consumption (gal/GGE) of Renewable Diesel via CAP Using the Displacement Method, Compared to 2.7 gal/GGE for Petroleum Diesel

The direct water consumption for the via acids pathway in the 2021 SOT case is 15.3 gal/GGE, which is comparable to the 15.4 gal/GGE in the 2020 SOT case. The direct water consumption for the via BDO pathway is 24.6 gal/GGE in the 2021 SOT case, which is the same as the 2020 SOT case.

3.5.3 Supply Chain NO_x Emissions

Total NO_x emissions from the 2021 SOT cases are 17% to 56% and 16% to 59% higher than petroleum diesel for the acids and BDO pathway designs, respectively, depending on the basis (mass or market value) used for the process-level allocation (Figure 33). Embedded emissions from manufacturing the process chemicals and catalysts required for the CAP conversion are the major emission source.

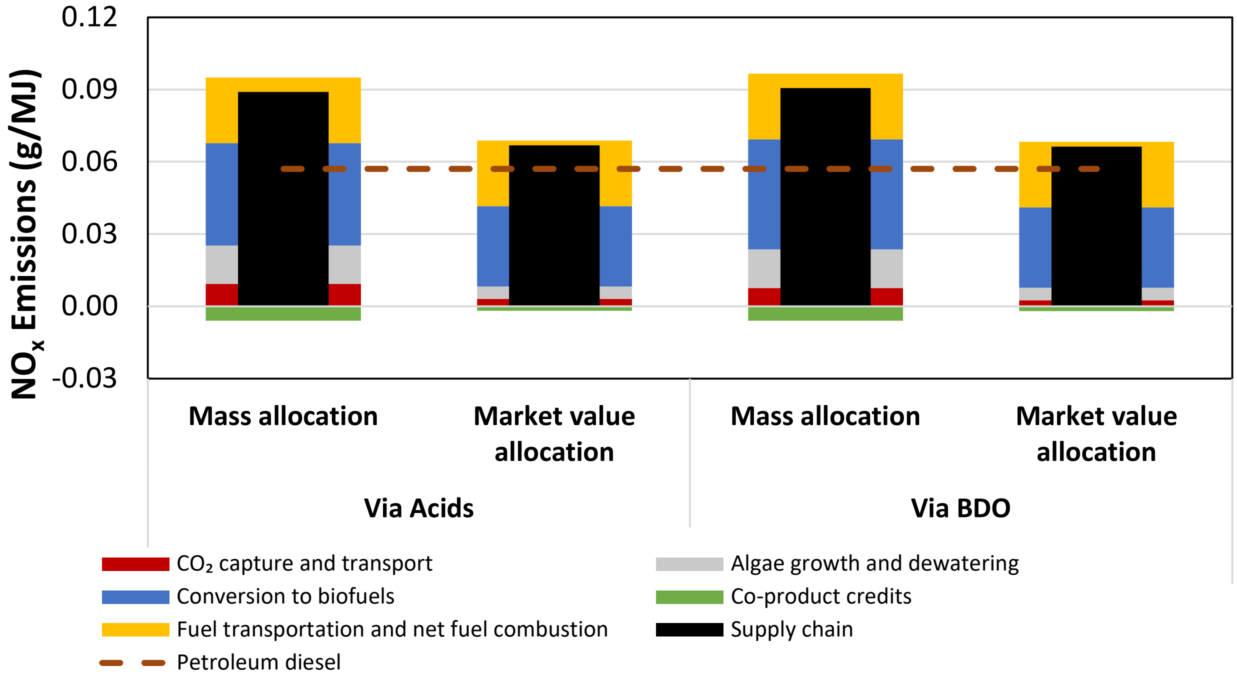


Figure 33 Supply Chain NO_x Emissions (g/MJ), Renewable Diesel via CAP Using the Process-Level Allocation Method, Compared to 0.06 g/MJ for Petroleum Diesel

Under the displacement method (Figure 34), embedded NO_x emissions from manufacturing the process chemicals and catalysts required for the CAP conversion are the major source of NO_x emissions. Other major drivers include NO_x associated with energy consumption for algae cultivation and dewatering and NO_x emissions during vehicle operation. The PU co-product generate a significant NO_x displacement emission credit from avoiding emissions from production of conventional fossil-based PU.

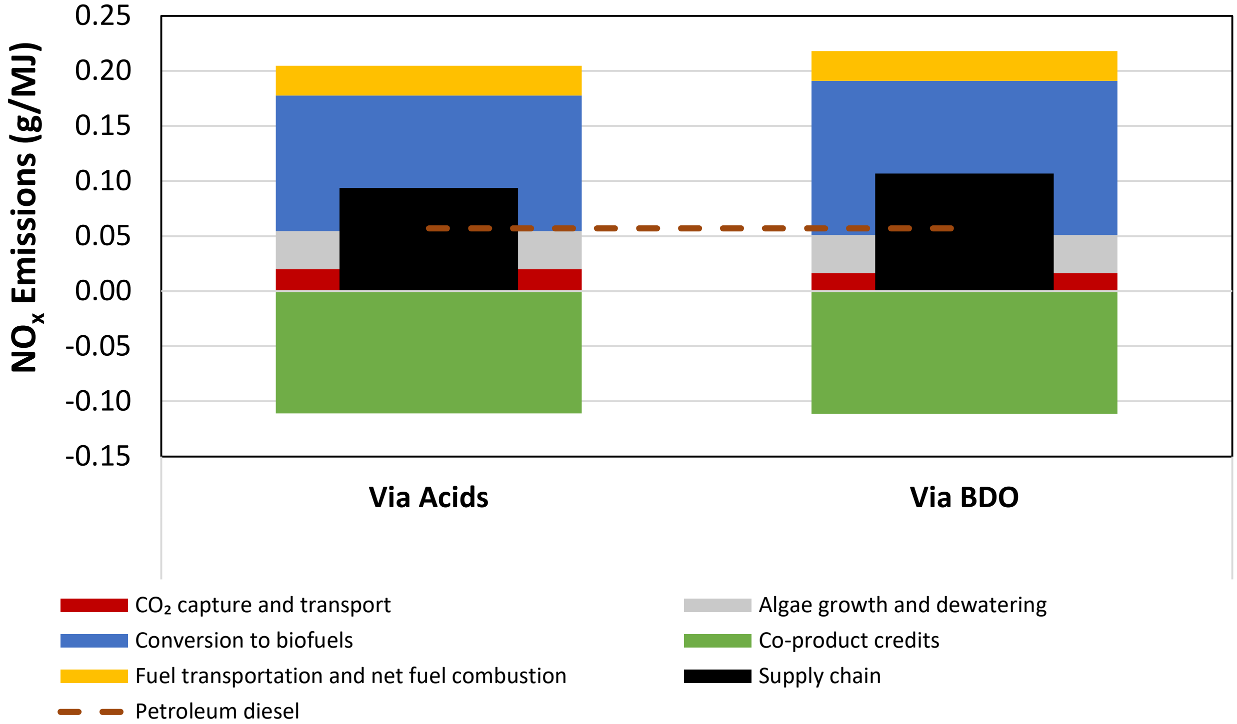


Figure 34 Supply Chain NO_x Emissions (g/MJ), Renewable Diesel via CAP Using the Displacement Method, Compared to 0.06 g/MJ for Petroleum Diesel

3.5.4 Summary of Sustainability Metrics

Tables 16 summarizes supply chain sustainability metrics, including fossil energy consumption, NEB, GHG emissions, water consumption, and NO_x emissions of RD from the CAP conversion designs in the 2021 SOT and future scenarios. Note that these results also consider the displacement credits of recycled nutrients, such as ammonia and diammonium phosphate from anaerobic digester effluent during the CAP conversion processes, which reduces makeup requirements of such nutrients in the algae cultivation phase. The basis on which the process-level allocation is performed has a great impact on the results because the PU co-product has much higher market value than the renewable diesel on a per-kg basis.

Table 16 Supply Chain Sustainability Metrics for Renewable Diesel via CAP, 2021 SOT Case

	Scenario 1: Via Acids		Scenario 2: Via BDO		
	Mass-based allocation	Market-value-based allocation	Mass-based allocation	Market-value-based allocation	Petroleum Diesel
			Biofuel yield		
mmBtu/dry ton	15.8	48.6	15.9	48.6	
			Co-product yield		
Power exported to grid, kWh/mmBtu of biofuel	21.7	7.1	22.0	7.2	
			Fossil energy consumption		
MJ/MJ	0.8	0.4	1.1	0.7	1.2
			Net energy balance		
MJ/MJ	0.2	0.6	-0.1	0.3	
			GHG emissions		
g CO_2e/MJ	59 (-35%)	34 (-62%)	74 (-19%)	48 (-47%)	91
g CO_2e/ GGE	7,214	4,199	9,048	5,866	11,157
			Water consumption		
L/MJ	0.94	0.78	0.63	0.45	0.08
gal/GGE	30.4	25.3	20.4	14.7	2.7
			Total NO_x emissions		
g NO_x/MJ	0.09	0.07	0.09	0.07	0.06
g NO_x/GGE	10.9	8.2	11.1	8.1	7.0
			Urban NO_x emissions		
g NO_x/MJ	0.03	0.02	0.03	0.02	0.03
g NO_x/GGE	3.1	2.6	3.1	2.7	3.3

Note: The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

Tables 17 summarizes the sustainability metrics for PU produced via CAP. In this analysis, we have updated our LCA results of conventional flexible foam PU (produced from toluene diisocyanate and polyether polyol) with detailed LCI of the PU production processes (Keoleian et al. 2012). Algae-based PU has 19% to 52% lower GHG emissions than conventional PU in the 2021 SOT case because it contains biogenic carbon, which comes from algae and generates a biogenic carbon sequestration credit. Algae-based PU has higher GHG emissions when market value-based, process-level allocation is used because more emission burdens are allocated to PU production, given its higher market value than that of the fuel on a mass basis.

Table 17 Supply Chain Sustainability Metrics for PU via CAP, 2021 SOT Case

	Scenario 1: Via Acids		Scenario 2: Via BDO		
	Mass-based allocation	Market-value-based allocation	Mass-based allocation	Market-value-based allocation	Conventional PU
			PU yield		
ton/dry ton	0.42	0.27	0.42	0.27	
			Fossil energy consumption		
MJ/kg	55.4	68.5	62.0	76.2	70.2
			GHG emissions		
g CO_2e/kg	2,005 (-38%)	2,940 (-10%)	2,378 (-27%)	3,364 (3%)	3,252
			Water consumption		
L/kg	18.4	24.5	19.6	26.3	4.8
			Total NO_x emissions		
g NO_x/kg	3.9	4.7	4.3	5.3	3.7

Note: The values in parentheses are the percentage of difference compared to the petroleum diesel pathway. Reduction is represented with negative values.

Table 18 summarizes supply chain sustainability metrics, using the displacement method.

Table 18 Supply Chain Sustainability Metrics for Renewable Diesel via CAP Pathways in the 2021 SOT Case, Using the Displacement Method

	Scenario 1: Via Acids	Scenario 2: Via BDO	Petroleum Diesel
		Biofuel yield	
mmBtu/dry ton	7.4	7.3	
		Co-product yield	
Polyurethane, kg/mmBtu of biofuel	27.8	27.8	
Power exported to grid, kWh/mmBtu of biofuel	46.7	47.6	
		Fossil energy consumption	
MJ/MJ	0.4	0.9	1.2
		Net energy balance	
MJ/MJ	0.6	0.1	
		GHG emissions	
g CO_2e/MJ	26 (-71%)	51 (-44%)	91
g CO_2e/ GGE	3,193	6,227	11,157
		Water consumption	
L/MJ	1.30	1.02	0.08
gal/GGE	42.1	33.1	2.7
		Total NO_x emissions	
g NO_x/MJ	0.09	0.11	0.06
g NO_x/GGE	11.5	13.1	7.0
		Urban NO_x emissions	
g NO_x/MJ	0.03	0.03	0.03
g NO_x/GGE	3.5	3.6	3.3

Table 19 summarizes biorefinery-level sustainability metrics for the algae CAP pathway. In the 2021 SOT case, the CAP biorefinery achieves reductions in fossil energy consumption and GHG emissions, but consumed more water due to makeup water requirements and the use of chemicals like corn steep liquor, which requires a large amount of water for its production. RD produced from CAP has lower GHG emissions than petroleum diesel in all the cases despite the basis for the process-level allocation method. PU production from CAP also contributes to the biorefinery GHG emissions reduction when compared to conventional PU production because of the sequestration of its biogenic carbon. Biorefinery NO_x emissions saw a slight increase relative to the conventional diesel and PU production.

Table 19 Biorefinery-Level Sustainability Metrics of Algae CAP, 2021 SOT Case

	Scenario 1: Via Acids		Scenario 2: Via BDO		
	Mass-based allocation	Market-value-based allocation	Mass-based allocation	Market-value-based allocation	

			Products		
Renew diesel	7.4		7.3		mmBtu/dry ton biomass
PU	0.2		0.2		ton/dry ton biomass
			Fossil energy consumption		
Direct consumption by RD production	6,154	3,476	8,589	5,674	MJ/dry ton biomass
Credits from RD production	-9,316	-9,316	-9,303	-9,303	MJ/dry ton biomass
Net consumption by RD production	*-3,162 (51%)*	*-5,840 (94%)*	*-714 (30%)*	*-3,630 (151%)*	MJ/dry ton biomass
Direct consumption by PU production	11,322	14,000	12,664	15,580	MJ/dry ton biomass
Credits from PU production	-14,354	-14,354	-14,354	-14,354	MJ/dry ton biomass
Net consumption by PU production	*-3,032 (49%)*	*-354 (6%)*	*-1,690 (70%)*	*1,226 (-51%)*	MJ/dry ton biomass
Net Total	-6,194		-2,403		MJ/dry ton biomass
			GHG emissions		
Direct emissions from RD production	457	266	573	371	kg/dry ton biomass
Credits from RD production	-707	-707	-706	-706	kg/dry ton biomass
Net emissions from RD production	*-250 (50%)*	*-441 (87%)*	*-134 (43%)*	*-335 (107%)*	kg/dry ton biomass
Direct emissions from PU production	410	601	486	687	kg/dry ton biomass
Credits from PU production	-665	-665	-665	-665	kg/dry ton biomass
Net emissions from PU production	*-255 (50%)*	*-64 (13%)*	*-179 (57%)*	*23 (-7%)*	kg/dry ton biomass
Net Total	-505		-312		
			Water consumption		
Direct consumption by RD production	1,929	1,601	1,291	929	gal/dry ton biomass
Credits from RD production	-169	-169	-169	-169	gal/dry ton biomass
Net consumption by RD production	*1,761 (70%)*	*1,432 (57%)*	*1,122 (58%)*	*760 (40%)*	gal/dry ton biomass
Direct consumption by PU production	995	1,324	1,058	1,420	gal/dry ton biomass
Credits from PU production	-257	-257	-257	-257	gal/dry ton biomass
Net consumption by PU production	*739 (30%)*	*1,067 (43%)*	*802 (42%)*	*1,163 (60%)*	gal/dry ton biomass
Net Total	2,499		1,923		gal/dry ton biomass
			Total NO_x emissions		
Direct emissions from RD production	691	519	702	514	g/dry ton biomass
Credits from RD production	-443	-443	-443	-443	g/dry ton biomass
Net emissions from RD production	*247 (87%)*	*75 (26%)*	*259 (67%)*	*71 (18%)*	g/dry ton biomass
Direct emissions from PU production	798	971	887	1,075	g/dry ton biomass
Credits from PU production	-761	-761	-761	-761	g/dry ton biomass
Net emissions from PU production	*37 (13%)*	*209 (74%)*	*126 (33%)*	*314 (82%)*	g/dry ton biomass
Net Total	285		385		g/dry ton biomass

Note: Positive net totals indicate net increases compared to conventional products. Negative net totals indicate net reductions compared to conventional products. The values in parentheses are contributions to the net totals by RD and co-product in percentage.

4 CONCLUSIONS

SCSAs of the 2021 SOT cases of five renewable diesel and renewable gasoline pathways are conducted. For pathways with significant co-product effects, we applied three co-product handling methods to address the co-product effects: a process-level allocation method, a displacement method, and a biorefinery-level analysis. Detailed SCSA results of the 2021 SOT case continue to track sustainability performance as ongoing research and development efforts aim to improve the technology readiness level and economic viability of these biofuel production pathways.

Producing HOG via IDL from logging residues in the 2021 SOT case yields a fuel that is 81% less GHG-intensive throughout its supply chain than conventional gasoline. GHG emissions from the biomass field preprocessing and depot preprocessing were the largest contributors to supply chain GHG emissions among the biomass logistics steps, while the energy-independent IDL process itself is a minor emission source. Research and development efforts to further reduce supply chain GHG emissions could focus on reduced consumption of process energy for biomass preprocessing and improvement of conversion yield. Although relatively water-efficient, the IDL process is the most water-intensive step in the supply chain and has the largest potential for further water consumption reduction for the pathway. The IDL process that combusts intermediate bio-char and fuel gas to meet process heat demand is the primary NO_x emission source, and thus NO_x emission control of this combustion source presents the greatest opportunity to mitigate supply chain NO_x emissions of the HOG via IDL pathway. HOG via IDL shows significant reduction potential in fossil energy consumption, as indicated by its NEB values of 0.79 MJ/MJ in the 2021 SOT case, owing mostly to the energy self-sufficient IDL to HOG process.

Producing RD via sludge HTL in the 2021 SOT case offers 78% and 83% GHG emission reductions with and without NH_3 removal, respectively. Supply chain water consumption is 2.3 gal/GGE and 1.8 gal/GGE with and without NH_3 removal, respectively. Fuel combustion and HTL for biocrude production are the primary contributors to NO_x emissions. With improvement in HTL energy efficiency, the design case has a slightly lower NO_x emission intensity than that of petroleum diesel. The sludge HTL pathway has a NEB of 0.73 MJ/MJ (with NH_3 removal) and 0.76 MJ/MJ (without NH_3 removal) in the 2021 SOT case.

SCSA results vary significantly with different co-product handling methods for those pathways that include significant non-fuel co-products. With the process-level allocation method, the supply chain energy and material requirement to produce the renewable fuels and non-fuel co-products are separated based on the design purposes and the relative ratios by mass or market value between the fuel and co-products. The displacement method considers impacts from both the fuel and non-fuel co-products, but attributes these overall impacts to the fuel product only. As a result, the SCSA results of the fuel product may be distorted by a significant displacement credit from the co-products. A biorefinery-level analysis, on the other hand, aims to provide a full picture of the sustainability impacts brought about by both the fuel and non-fuel co-products and sheds light on the overall sustainability of the biorefinery in comparison to incumbent technologies and products.

For the biochemical conversion pathway producing BKA as a co-product from lignin upgrading, taking the supply chain GHG emissions as an example, the conversion step is the primary GHG emission source in the 2021 SOT case, owing to large quantities of process chemicals and energy required for pretreatment operations. In the lignin upgrading to BKA case and with the process-level allocation method, the supply chain GHG emissions are 19% to 43% higher for the 2021 SOT acids and BDO intermediate pathways, respectively, than those of the petroleum diesel. On the other hand, supply chain GHG emissions are 5% lower and 23% higher for the 2021 SOT acids and BDO intermediate pathways, respectively, than those of the petroleum diesel, when the co-product BKA is handled with the displacement method, assuming conventional NG-derived AA is displaced. In either case, the supply chain GHG emissions are projected to improve relative to these SOT benchmarks based on future 2030 performance goals.

RD biofuel produced from HTL of WWTP-cultivated algae offers a 107% reduction in GHG emissions in the 2021 case compared with those of petroleum diesel. The great reduction is because the waste-derived algae feedstock does not require external nutrients to grow and does not consume much external energy to dewater to a desired solid content of 20%. On the other hand, the struvite co-product generates credits by displacing synthetic N and P fertilizers, which also helps to achieve low life-cycle GHG emissions, water consumption, and NO_x emissions. The combination of waste-derived algae feedstock and struvite co-product credit also helps the algae HTL pathway to achieve great reductions in supply chain water consumption and NO_x emissions in the 2021 SOT case compared to petroleum diesel.

When the process-level allocation method is applied, the algae CAP pathway has 19% to 35% (mass-based allocation) and 47% to 62% (market value-based allocation) lower GHG emission intensities in the 2021 SOT case, compared to petroleum diesel. Water consumption remains higher for the CAP pathway even when saline algae species are reflected, because of significant embedded water consumption associated with the process chemical and catalyst use for fuel production operations, as well as water consumption associated with electricity demands for algae cultivation and dewatering. Reducing process chemical and energy requirements and improving algae biomass productivity and algal fuel yield would be key to mitigating the sustainability impacts including GHG emissions, water consumption, and NO_x emissions. With the displacement method, the GHG emission intensity of the fuel is about 44% to 71% lower in the 2021 SOT case than that of petroleum diesel. At a biorefinery-level, 0.34 to 0.56 tons of GHG emission reduction per ton of biomass converted to fuel and PU products would be expected.

Finally, biomass-derived chemical co-products in integrated biorefineries tend to offer significant carbon reduction potential, compared to conventional counterparts that use fossil feedstocks to produce. It is an important contribution to the overall biorefinery-level carbon reduction potential and should be considered together with potential carbon emission reduction potentials of biofuels.

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