



Life cycle environmental and cost evaluation of renewable diesel production

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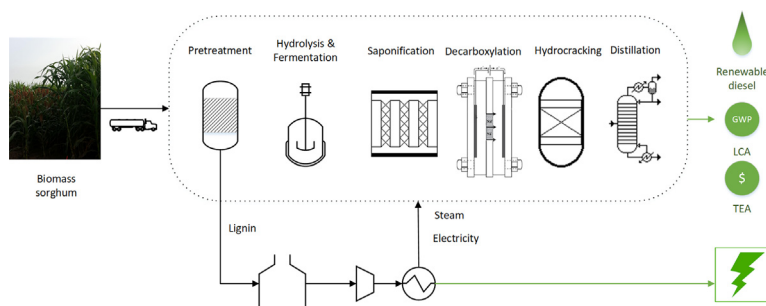
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GRAPHICAL ABSTRACT



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ABSTRACT

Computer simulations are used to study the production of renewable diesel through the biochemical transformation of biomass sorghum [*Sorghum bicolor* (L.) Moench] to free fatty acids using a genetically modified strain of *Escherichia Coli*. We evaluate select environmental and economic metrics using life cycle assessment (LCA) and techno-economic analysis (TEA). The biofuel supply chain includes feedstock production, handling, pretreatment and hydrolysis, fermentation to free fatty acids, saponification of the free fatty acids, wax production on an electrochemical synthesis reactor, and hydrocracking to convert the wax to renewable diesel. The TEA model developed uses experimental data from pretreatment to wax synthesis steps and literature for the conversion of wax to diesel. The TEA model is integrated into a life cycle inventory model to estimate life cycle greenhouse gas and non-renewable energy consumption. Considering both environmental and economic factors we find that the performance of this pathway to produce renewable diesel returns lower product yield, higher cost, and higher GHG and energy impacts compared to biomass-to-ethanol pathways, primarily due to poor process yields (mainly fermentation). This limitation in the metabolic pathway constrains the maximum yield potential of FFA and therefore renewable diesel and other potential co-products from biomass derived sugars.

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1. Introduction

The ever-increasing demand for and environmental impact of petroleum-based transportation fuels require the identification of novel sources of low-carbon alternatives. Numerous renewable energy strategies are currently being investigated including solar energy, wind, and ethanol or infrastructure compatible fuels from biomass. While many of these alternatives have potential for reducing our dependency on fossil fuels for short haul ground transportation, long haul transportation, both air and ground, will continue to depend on infrastructure compatible hydrocarbon fuels. The energy density of batteries and even alcohol fuels is low for any application where range and payload are important, such as long-haul trucking and rail shipping. Therefore, it is important to develop renewable diesel to positively impact the long-haul transportation sector.

Renewable diesel is a non-oxygenated fuel derived from a process that involves the conversion of feedstock material or fatty acids into straight chain n-alkanes through deoxygenation, which can be further processed to meet the specifications of renewable diesel fuel. Renewable diesel does not have double bonds or oxygen, which increases the energy content of the fuel relative to biodiesel. It also presents low viscosity, absence of sulfur, and a production process flexible enough to allow the production of different hydrocarbon fuels that can meet most fossil fuel specifications [1]. Due to these characteristics renewable diesel is a promising infrastructure compatible or “drop-in” fuel. The expected expansion of long-haul transport fuel markets further motivates the development of renewable diesel [2]. In most prior studies, production of renewable diesel has been considered by catalytic hydrotreating of vegetable oils, Fischer Tropsch synthesis or upgrading of pyrolysis bio-oil using biomass derived syngas [3].

In this work, renewable diesel is made from the deoxygenation of fatty acids. We analyze the use of a new technology for the decarboxylation pathway (in which oxygen is removed as carbon dioxide) using an electrochemical reactor studied previously using ready sources of free fatty acids from waste sources [4]. Free fatty acids can be derived from animal, plant or vegetable oils but their use for renewable diesel production could lead to a shortage of edible oils, which may interfere with food prices [5]. The use of animal fats, used fried oils and waste oils as feedstock could help reduce production costs, but those resources are limited and might not be sufficient to satisfy the increasing demand for renewable fuels [6]. An alternative to this process is the biological transformation of lignocellulose to free fatty acids, which are naturally accumulated in most oleaginous microorganisms and can be and are used in the production of biofuels (biodiesel) or biochemicals [7,8].

Lignocellulosic feedstocks are a promising raw material for biofuel production, and include agricultural residues, cellulosic waste, and herbaceous and woody crops. They have several advantages including that they are abundantly available and they do not compete with food production or animal feed [9–11]. Herbaceous energy crops such as switchgrass and biomass sorghum can grow on soils not suitable for alimentary crops; they can reduce soil erosion, increase water quality and have a positive impact on wildlife [12,13]. Thus, the production of renewable diesel from agricultural biomass could have environmental benefits much greater than their economic benefits.

Computer simulations have been used successfully to model and predict the material and energy consumption of many industrial processes. They provide the ability to estimate the effect of variations in raw material, changes in operational conditions, process configurations or incorporation of new technology, including for biomass and biofuels [14]. Various authors have reported models for fuel ethanol production from different feedstocks using well-known process software such as SuperPro Designer® (Intelligen Inc., Scotch Plains, NJ) [15] and Aspen Plus® (Aspen Technologies Inc., Cambridge, MA) [16–18]. These simulations provide material and energy balances that have been used as the basis for techno-economic and environmental life cycle evaluations of different production processes, including for the production of

ethanol [19], fatty acid ethyl esters [20], renewable diesel [21] and bio-jetfuel blendstock [22–24] produced from biochemical and thermochemical conversion processes. In this work we use computer simulations to study the production of renewable diesel through the biological transformation of biomass sorghum [*Sorghum bicolor* (L.) Moench] to free fatty acid [25] and thence electrochemical decarboxylation to a bio-wax that undergoes hydrocracking to renewable diesel. Biomass or energy sorghum is a highly productive drought tolerant C4 photosynthetic species that is amenable to current annual cultivation systems in the U.S. [26] and one that the U.S. Department of Energy has identified as the key annual energy crop [27]. Annual crops fit well into existing crop rotation systems and provide additional insurance to biomass supply if stand failure occurs unexpectedly in a perennial crop. Under large plot dry land conditions, current sorghum cultivars can produce between 15 and 25 dry Mg ha⁻¹ [26]. Unlike perennial energy crops, annual cropping lowers risks to growers due to short-term investment and the presence of alternate animal feed markets, which have motivated its study for deployment within the continental U.S. [28]. We evaluate select environmental and economic metrics using life cycle assessment (LCA) and techno-economic analysis (TEA). Prior LCA study of forage sorghum [29] examined the life cycle environmental tradeoffs of irrigated crop production in California. Gnansounou et al. [30] used TEA to evaluate alternative configurations of sweet sorghum production in China; and Adler et al. [31] combined LCA and TEA to evaluate greenhouse gas (GHG) abatement costs of ethanol produced from grain and sweet sorghum crops in Uruguay as a gasoline substitute. Our objective is to evaluate the impact of select life cycle environmental and economic metrics of converting biomass sorghum to renewable diesel, an infrastructure compatible fuel that could qualify as an advanced fuel under the U.S. Renewable Fuel Standard, RFS2 [32]. We evaluate biomass sorghum production in the Texas-gulf region where yield potential and economics favor its production [33] and due to proximity to petroleum processing infrastructure, including pipelines, refineries and blending facilities; however, production may extent to a greater growing area on current and potential future cropland and pastureland [28].

2. Methods

We use chemical process modeling and simulation in Aspen Plus® (Aspen Technologies) to predict conversion yields and process economics, and develop material and energy balances as a basis for the biofuel conversion step in the LCA of biomass sorghum-to-renewable diesel. We adapt our process modeling work from the model developed by the National Renewable Energy Laboratory (NREL) for the biochemical conversion of corn stover to ethanol, using dilute-acid pretreatment and enzymatic hydrolysis of corn stover [34] to represent the renewable diesel production process. We describe each step in the biofuel conversion process model (Fig. 1) that is divided into nine major areas from initial intake of feedstock (A100) to product and process chemical storage (A700) and energy and utilities (A900).

Feedstock handling (A100): Biomass sorghum enters the biorefinery with known, uniform specifications (particle mean size of 0.41–0.58 cm, mean bulk density of 144–176 kg m⁻³, 20% moisture) following processing at a central depot as specified for a pioneer uniform-format feedstock supply system [35]. The feedstock composition (Table 1) entering this area undergoes weighing, storage and distribution.

Pretreatment (A200): The plant processes 500 dry metric tons per day (MTPD) of biomass sorghum, this capacity was determined to represent a realistic supply of the raw material in the Texas-gulf region suitable for growing the feedstock. The biomass sorghum is treated in a reactor in order to liberate the cellulose and hemicellulose from the lignin seal and its crystalline structure. We model an alkaline pretreatment that uses 18 mg NaOH g⁻¹ dry biomass at 120 °C, a residence time of 5 min and 15% solids, according to results from sugars obtained

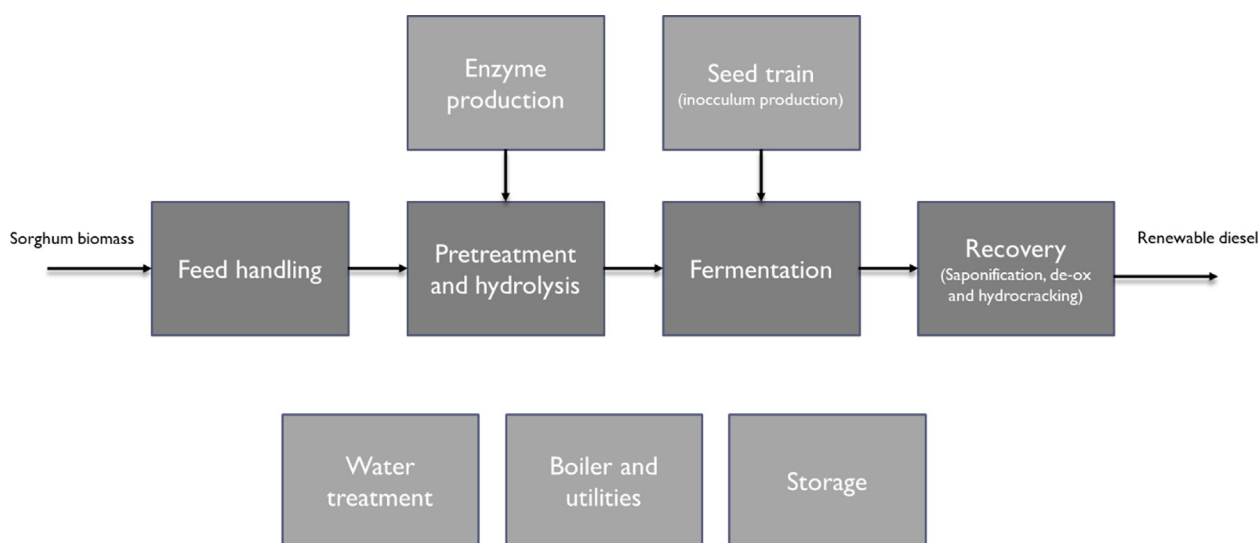


Fig. 1. Diagram of the simulated process.

Table 1
Sorghum biomass composition considered in simulations.

Component	Content (%)		Source
	Range	Value used (%)	
Water		20	(Humbird et al. 2011) [34]
Extractives		16.89	Assumed to close mass balance
Sucrose	0.3–19	9.0	(Stefaniak et al. 2012) [36]
Glucan	21.7–37.7	29.1	(Stefaniak et al. 2012) [36]
Galactan	0.8–1.2	1.0	(Dahlberg et al. 2011) [37]
Mannan	–	–	
Xylan	11.9–20.7	16.4	(Stefaniak et al. 2012) [36]
Arabinan	2.1–3.0	2.5	(Dahlberg et al. 2011) [37]
Lignin*	8.9–20.6	13.7	(Stefaniak et al. 2012) [36]
Acetate		1.81	(Humbird et al. 2011) [34]
Protein	0.6–5.2	3.3	(Stefaniak et al. 2012) [36]
Ash	2.3–9.9	6.3	(Stefaniak et al. 2012) [36]
Starch	0.0–12.0	5.6 ¹	(Stefaniak et al. 2012) [36]

¹ Included as extractives for modelling.

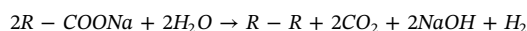
from switchgrass feedstock by Lee et al. [38].

Hydrolysis and Fermentation (A300): In the hydrolysis step enzymes convert cellulose and hemicellulose molecules to C5 and C6 monomers in a continuous reactor operating at 15% total solids loading, 50 °C and 20 mg protein/g glucose of cellulase loading. The hydrolyzed slurry is then sent into a series of parallel batch fermenters where a micro-organism is added to convert the monomeric sugars into free fatty acid. We use *Escherichia coli* strain *ML190(pXZ18Z)* at 30 °C, its yields transforming sugars derived from woody hydrolysate into free fatty acids are described by Wu et al. [39]. We defined the stoichiometry of the fermentation reactions based on the maximum theoretical yield of each free fatty acid from the correspondent sugar, calculated by [40] by constraint based modelling. Maximum theoretical yields are 0.34 g/g for both palmitic and myristic acid from glucose, and 0.28 g/g and 0.29 g/g for palmitic and myristic acid respectively from xylose. While these yields are lower than yields associated with ethanol (0.51 g/g from both glucose and xylose), there is only 15% oxygen in fatty acids from carbohydrates whereas ethanol has 35% oxygen. Thus, the total energy content is comparable by HHV.

Based on experimental results from Mosby et al. [41], the composition of the FFAs is roughly 40% palmitate and 55% myristate, < 5% other; thus, we modelled the FFA as 60% myristate and 40% palmitate. Between hydrolysis and fermentation the total residence time for this stage is 7 days.

Enzyme production (A400): In this stage the cellulase enzyme necessary for the hydrolysis is produced using *Trichoderma reesei*, a filamentous fungus that secretes high levels of cellulase enzymes when grown aerobically in the presence of cellulase inducers.

Wax and diesel production (A500): This stage comprises all the process units necessary to convert the free fatty acids into diesel. The fermentation goes through a centrifuge that separates solids from liquid, the solids go to the boiler (A800) and the stream containing free fatty acids is concentrated in a second centrifuge to achieve 10% (w/v) of free fatty acids, before entering a saponification reactor. In this plug flow reactor, 100% of each free fatty acid is converted into its respective sodium salts. Sodium salts enter an electrochemical reactor [41] that convert the sodium salts into wax. It uses a catholyte solution of water and sodium hydroxide (that is recycled into the saponification reactor), an anolyte solution with 40% methanol, and 60% water with sodium salts from the saponification reactor. It uses a NaSICON membrane with a cell voltage of 6 V at 100 mA/cm², the reaction that occurs is:



According to Liu et al. [42] the selective hydrocracking of Fischer-Tropsch (F-T) waxes to diesel-ranged hydrocarbons (C₁₁–C₂₀) is considerably more difficult than the selective hydrocracking of F-T waxes to gasoline-ranged hydrocarbons (C₅–C₁₀) due to the further cracking of C₁₁–C₂₀ hydrocarbons. Hydrocracking products are very dependent on the feed and on the catalyst used for this process. No experimental information is yet available for the conversion of our wax to diesel, therefore we used data from Kobayashi et al. [43] that uses a Fischer-Tropsch wax named FTW-1. Its carbon number distribution, is similar to the experimental results obtained for our wax (C₂₆–C₃₀). Diesel yield from this wax was 42% on a mass basis.

The wax is converted to renewable diesel via hydrocracking according to Kobayashi et al. [43] followed by fractionation by crude distillation. The cetane index of the obtained diesel can be estimated to be larger than 95, following the procedure in Kobayashi et al. [44] based on the average carbon number and the paraffin content. Heating utilities and steam consumption for the distillation step are based on the work of Ji and Bagajewicz [45] on a conventional crude distillation unit with heat integration. Further, commercial processes to convert lipids into drop-in diesel fuel constitute catalytic deoxygenation using hydrogen at high pressure and temperature. Hydrogen can only be economically produced at large scale suitable for feeding a petroleum refinery sizes. Our pathway removes oxygen from biomass derived fatty acids via decarboxylation, a process independent of hydrogen. Two

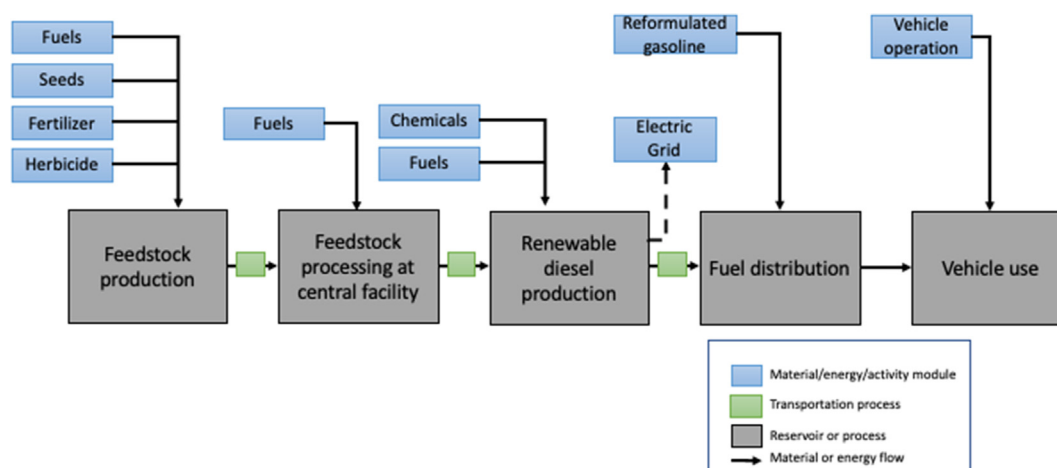


Fig. 2. Life cycle framework for renewable diesel production from lignocellulosic material.

moles of oxygen are removed by C–C bond cleavage rather than hydrogen via hydrodeoxygenation. Since hydrogen is not an input in our process, the eventual commercialization can be performed at smaller distributed scales.

Wastewater treatment (A600): Wastewater streams from the facility are treated by anaerobic and aerobic digestion. The biogas produced in the anaerobic digester is sent to the combustor, (Area 800). After treatment, the water is suitable for recycling and is returned to the pretreatment area (Area 200).

Combustor, boiler, and turbogenerator (A800) and utilities (A900): The solids from the first centrifuge (A500) and the biogas from anaerobic digestion (A600) are burned in a fluidized bed combustor to produce high-pressure steam for electricity production and process heat. If the boiler produces excess steam, it is converted to electricity for use in the plant and for sale to the grid as a co-product. All utilities, including cooling water, chilled water, process water, and power are found in section A900 of the biorefinery.

3. Process economic analysis

Variable operating cost: The variable operating costs are obtained using the material and energy balance calculations of the Aspen Plus simulations and expressed in USD. The materials include biomass sorghum at \$68.84 dry metric ton⁻¹, pretreatment and neutralization chemicals, nutrients (corn syrup liquor and potassium salts), wastewater treatment chemicals and polymers, and diammonium phosphate. Table S8 in the Supporting information (SI) file documents feedstock delivered cost parameters based on assumed production on available pasture and hay lands for growing sorghum within a 160 km radius of West Lake, LA, the proposed site for the 500 dry MTPD biorefinery. Cost were adjusted to 2018 US\$ and align with cost ranges estimated by U.S. DOE [27]. Utilities include steam, power, water and hydrogen, the cost of hydrogen was \$4.49 kg⁻¹ [46]. Costs of the other materials and utilities were obtained from Humbird et al. [34].

Fixed operating cost: Labour cost was estimated from NREL's 2011 design basis [34], considering the degree of automatization of each process and salary guides. A factor of 90% applied to labour burden to cover safety, general engineering, general plant maintenance, payroll overhead, plant security, custodial and similar services, phone, light, heat, and communications. Annual maintenance cost was estimated at 3% of the total project investment, and property insurance and local property tax were estimated at 10.7% of the total project investment based on NREL's 2011 design basis [34].

Equipment cost and installed cost: Equipment is sized according to the material and energy balance calculations of the Aspen Plus simulations. Equipment costs are obtained from several sources, including past

vendor quotations from the corn stover ethanol biochemical design report [34], costing estimates from study updates in refinery investment cost for crude distillation [47] and hydrogen production, from information on hydrogen management in refineries [48] for hydrogen recovery and Guthrie's correlation [8] for the methane recovery distillation column. The capital cost of the electrochemical reactor was estimated as \$5.2 million by the Ceramtec design team. When the costs were derived from the NREL 2011 design case we used the power law to adjust for changes in capacity with the scaling exponent for the power law obtained from the NREL 2011 design case [34] for most of the equipment, NREL factors were also used to obtain the total project investment from the purchased equipment costs.

Discounted cash flow analysis: Discounted cash flows are used to determine the minimum renewable diesel selling price (MSP) that generates a net present value of zero for a 10% internal rate of return. The assumptions made for the discount flow analysis are: 40% equity financing and a 3-year construction period, a 30-year plant life, 35% federal tax rate and working capital is 5% of fixed cost investment. The cost year used is 2018 (real US dollars). Equipment quotations obtained in earlier or later years would be inflated or deflated to year 2018 using chemical indices.

4. Environmental life cycle assessment

We apply life cycle inventory (LCI) analysis according to ISO 14040 [49] methods to investigate the greenhouse gas (GHG) emissions in the biomass sorghum-to-renewable diesel life cycle (Fig. 2). The functional unit applied is 1 MJ of renewable diesel production, over a 20-year biorefinery lifetime. Inputs across the life cycle of the fuel include production and collection of feedstock; feedstock transport from the farm to the biorefinery; the bioconversion steps pretreatment and conditioning of feedstock, enzymatic hydrolysis and fermentation, wax production and refining. Steam and electricity are produced onsite by integrating a boiler that takes the high lignin fermentative by-product and converts it to electricity, as a co-product. If the energy generated is insufficient for the process, electricity is purchased and delivered. The cradle-to-gate inputs to the biorefinery are inventoried based on the Aspen Plus model. Material and energy consumption and production are shown in Tables S1 and S2 in the SI file. Carbon sequestration due to land use change was not included due to insufficient data; this is part of on-going research (e.g., see [50]). Inputs for fuel transportation and distribution are shown in Tables S3 and S4 of the SI.

Process Scenarios: To study the sensitivity of the overall yield of the process on the economics and environmental metrics of the process two cases were analyzed. The "state of the art" case, where all the yields are obtained either from previous published research or from information

on ongoing research by the authors of this paper and the “optimal case” in which all the yields are improved to 95%, which is deemed the likely highest attainable yield for all sub-processes between pretreatment, enzymatic hydrolysis, fermentation, decarboxylation, and wax hydrocracking.

5. Results and discussion

Process economics: The total capital investment (TCI) for the 500 dry MTPD biorefinery is \$339.7 million (7.2 2018 USD L⁻¹) with an operating cost of 5.13 2018 USD L⁻¹ (19.41 USD gallon⁻¹) for the state of the art renewable diesel and a \$353.6 million TCI (2.2 2018 USD L⁻¹) with an operating cost of 1.60 2018 USD L⁻¹ (6.03 USD gallon⁻¹) for the “optimal case” renewable diesel. Compared to prior research by Humbird et al. [34] on ethanol produced from corn stover, whose TCI for a 2000 MTPD facility is \$422.5 million (0.2 2007 USD L⁻¹) our estimated capital cost for production of drop-in fuels is 17%–20% lower but with a smaller capacity. Considering the capital cost per liter of fuel, investment in the renewable diesel facility should be diminished. The operating cost for corn stover-to-ethanol is 0.4 2007 USD L⁻¹ (1.25 USD gallon⁻¹) of ethanol produced, considerably lower than the cost of renewable diesel (5.1 2018 USD L⁻¹ in the base case and 1.6 2018 USD L⁻¹ in the state of the art case), which is largely due to the yields of the renewable diesel process being smaller, 0.021 kg diesel/kg feedstock for the “state of the art” and 0.07 kg diesel/kg feedstock for the “optimal case”, compared with the 0.208 kg ethanol/kg feedstock estimated by Humbird et al. [34] for corn stover-to-ethanol. Difference in yields cannot be overcome by higher efficiencies as the metabolic pathways limit the maximum yield potential of FFA and accordingly the quantity of renewable diesel produced. According to the values estimated by Lennen and Pfeleger [40], maximum theoretical yields for FFA production are 55%–67% of the yield for ethanol production from the same sugars, and more conversion steps are needed in order to obtain the biofuel, while ethanol is ready for distillation.

Nevertheless comparing water immiscible fuels that blend with petroleum-based fuels, such as renewable diesel, with ethanol, cost is not the only factor to consider, as there are documented obstacles to expanding the use of ethanol beyond current levels due to fuel distribution infrastructure and vehicle incompatibilities [20]. Stroger et al. [51] estimate a high marginal cost and consumption of diesel for ethanol transportation and distribution from producers in the U.S. Midwest to distant consumers in large population centers given the 10% ethanol blend wall, costs that amount to approximately \$0.03 L⁻¹ (\$0.12 Gal⁻¹) ethanol. Such cost savings should be reflected in the minimum selling price of the renewable diesel.

A cost reduction of \$8.5 L⁻¹ (\$32 gallon⁻¹) is observed when all stages of the process are improved to achieve high yields. The minimum selling price estimated for renewable diesel ranges from \$3.8 to \$12.3 L⁻¹ (\$14 to \$47 gallon⁻¹) depending on the yields considered for the different stages, the lower value is close to the \$2.50 L⁻¹ (\$9.58 L⁻¹) obtained by Davis et al. [52] for algal lipids and is significantly higher than the current price of diesel, which is approximately \$0.6 L⁻¹ [53]. The option to produce lubricant could improve the economy of the process, but as the MSP of renewable diesel is always greater than the actual selling price of lubricants at approximately \$1 L⁻¹ (\$4 gallon⁻¹), there is no amount of lubricant production that could make this process economically viable under the conditions we examine. Even in the best case, the MSP is higher than the current price of diesel, therefore it is necessary to analyze how costs are distributed in order to identify opportunities for cost reduction (see Fig. 3).

Fig. 3 shows that the greatest contributions to the selling price of the fuel are the capital recovery charge and raw materials (feedstock) costs; therefore, working with residues as raw materials and changing the process to reduce capital costs are good strategies to reduce the minimum selling price of the renewable diesel in order to reach a competitive price. The distillation and solids recovery stage has a high

capital cost, mostly due to the cost estimated for the electrochemical reactor and the hydrocracking unit. Reducing the electrochemical reactor cost, which is at the development stage, would also reduce total capital costs.

6. Life cycle assessment

Life cycle GHG emissions (Table 2) for renewable diesel cases are both lower than the value for low sulfur diesel, which is approximately 91 g CO₂e MJ⁻¹ noted in prior literature [54], but higher (for the optimal/95% yield case) than estimates found for lignocellulosic ethanol production in previous research. For example, Fertitta-Roberts et al. [29] estimate biomass sorghum-to-ethanol GHG emissions for E85 fuel to range from 29 to 44 g CO₂e MJ⁻¹. This range depends greatly on nitrogen management for the biomass sorghum crop. This is equivalent to ~38–59 g CO₂e MJ⁻¹ for the ethanol portion, given that the blend consists of 81% ethanol/19% gasoline by volume [55]. Adler et al. [31] estimate that GHG emissions for ethanol from grain and sweet sorghum, both first generation energy crops, can be as low as 20 and ~3 g CO₂e MJ⁻¹, respectively, values that are well below RFS2 GHG reduction targets for advanced biofuels. Those low GHG emissions intensities for grain and sweet sorghum depend upon agricultural land used for production, LCA framework (consequential or attributional) and method of estimating soil GHG emissions. They are also mature technologies with high ethanol yields. Lignocellulosic ethanol from corn stover has a lower GHG intensity range, 36–41 g CO₂e MJ⁻¹, compared to the 95% yield renewable diesel case and varies depending on how lignin residuals are used as co-products and how credits are estimated [56]. For lignocellulose feedstock, most of the difference in values (as with the economic results) can be explained by the difference in the process yields: 1.2 MJ kg⁻¹ feedstock for the “state of the art” and 4.0 MJ kg⁻¹ feedstock for the “optimal case” (calculated with a LHV of 43.6 MJ kg⁻¹ diesel), compared with the 6.0 MJ kg⁻¹ feedstock for lignocellulosic ethanol. Life cycle findings show a need to reduce chemical and nutrient inputs to meet U.S. policy objectives, which is consistent with findings from previous research related to GHG emissions from enzymes and process chemicals [19,57]. Higher process yields in the 95% scenario lead to less “unused” biomass residuals sent to the boiler, and higher energy requirements in the separation and recovery steps, resulting in the need to purchase electricity from the grid, while the lower yields in the state of the art case lead to enough energy generated to satisfy process needs and sell the excess to the grid, which translates to an electricity credit. Similar observations were made for lignocellulosic ethanol when comparing high fermentation yields compared to state-of-the art fermentation [19].

Considering this distribution there is an opportunity to reduce GHG emissions with better technology for feedstock harvest and nutrient input, for example through implementing best management practices [63], and reducing the consumption of sodium hydroxide (Fig. 4). Future research should analyze the effect of changes in process stages (e.g., alternative pretreatment methods such as dilute acid rather than alkaline) and the production of co-products (e.g. lubricants) that can generate CO₂ credits. Summarizing, renewable diesel could be produced with the current process efficiencies at a cost of 12.3 2018 USD L⁻¹ and with an associated GHG emissions intensity of 21.4 g CO₂e MJ⁻¹ diesel. Improvement of processes efficiencies could reduce costs up to 3.8, but with higher GHG emissions of 69.3 g CO₂e MJ⁻¹ diesel. Considering these environmental and economic factors we find that the performance of the processes evaluated to produce renewable diesel is significantly lower than that of ethanol production processes for all metrics considered, primarily due to poor process yields (mainly fermentation). This limitation in the metabolic pathways constrain the maximum yield potential of FFA and therefore renewable diesel and other by-products from biomass derived sugars. Similar results were obtained for fatty acid ethyl esters FAEE production from switchgrass [20].

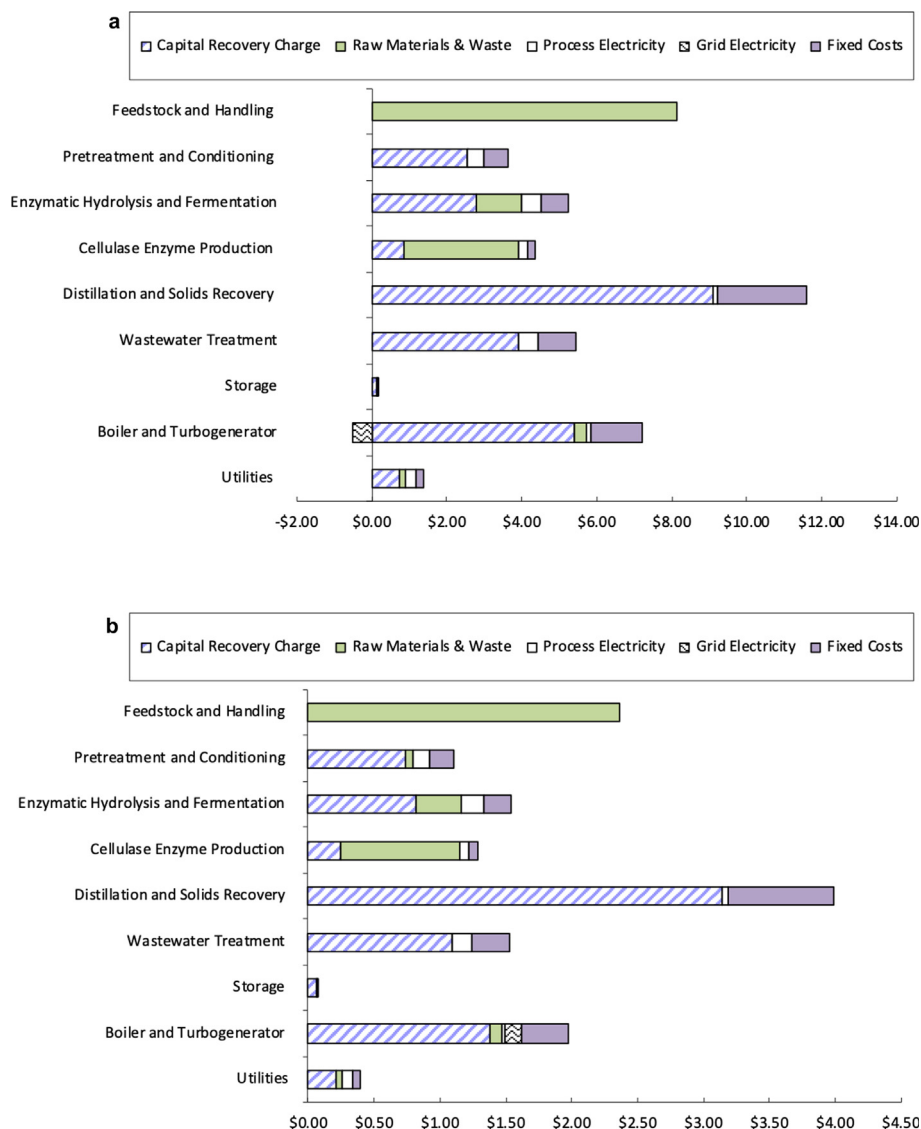


Fig. 3. Cost contribution details from each process area (per liter of diesel) for a) state of the art process b) 95% yields.

Table 2

GHG emissions of life cycle components: Feedstock production, feedstock transport, and fuel conversion for the state of the art and 95% yields.

Life Cycle Components	Model or Data Source	GHG emissions g CO ₂ e MJ ⁻¹ diesel	
		State of the art process	95% yields
Feedstock Production and transport:			
Crop establishment (lasting 11 years) and harvesting	Lerkkasemsan and Achenie (2013) [58]	4.4	1.3
Nutrient addition	Rooney [59]	18.1	5.2
Total soil N ₂ O emissions	1.5% of N-fertilizer applied	9.4	2.7
Biogenic carbon	Aspen Plus feedstock input	-1290.2	-368.6
Transport	SimaPro 8.4 [60]	12.2	3.5
Particle reduction	Bitra et al 2009 [61]; SimaPro 8.4 [60]	27.8	7.9
Fuel Conversion:			
Chemicals and Nutrients	Aspen Plus simulation, SimaPro 8.4 [60]	82.1	23.5
CO ₂ emissions	Aspen Plus simulation, SimaPro 8.4	1247.2	371.1
Electricity input	Aspen Plus simulation; SimaPro 8.0 [60]	0	21.3
Co-product (electricity)	Aspen Plus simulation; SimaPro 8.0 [60]	-91.1	0
Fuel transport & distribution	GREET 1 [62]	1.5	1.5
Total		21.4	69.3

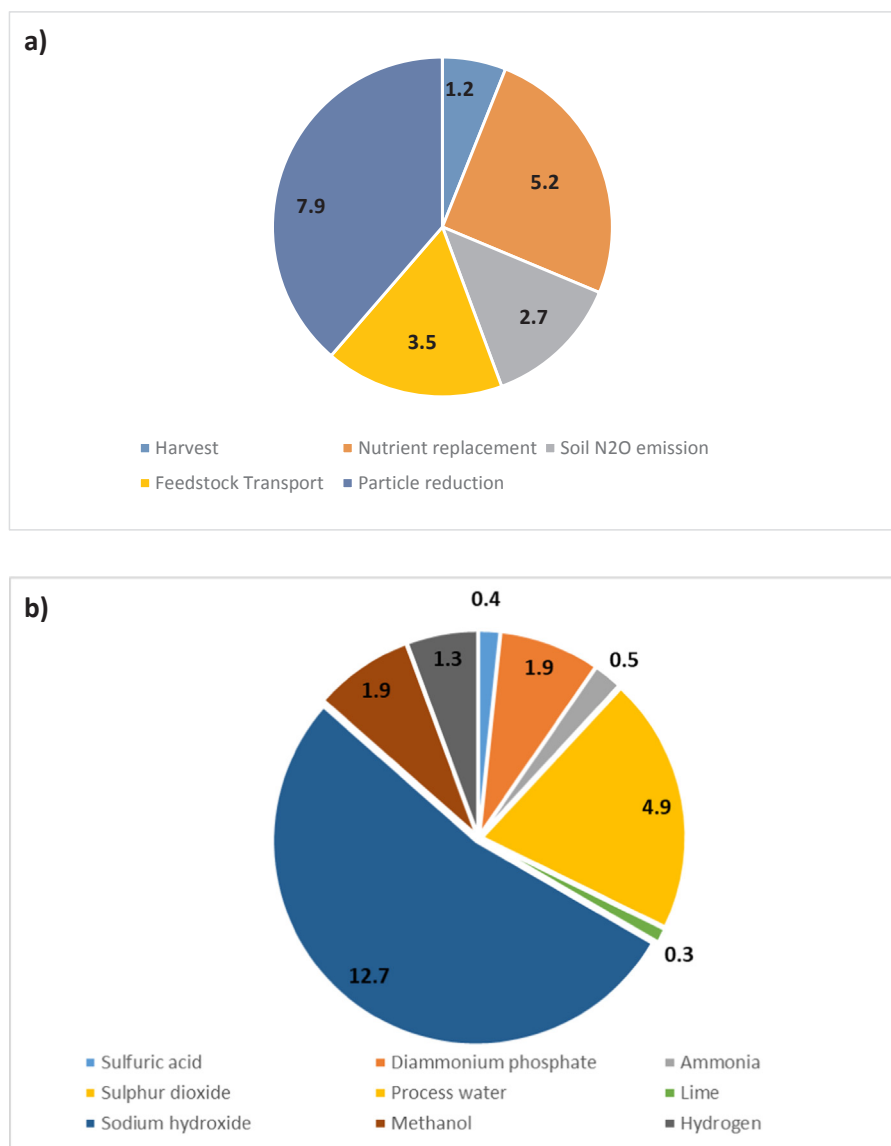


Fig. 4. Distribution of GHG emissions (g CO₂/MJ diesel) on a) Feedstock production and transport b) Chemicals and nutrients for the 95% yields.

7. Conclusions

Experimental data were combined with process modeling and simulation to estimate cost and a life cycle inventory for converting biomass sorghum to renewable diesel, an advanced drop-in biofuel. Although infrastructure compatible fuels like renewable diesel are foreseen to meet expanding liquid fuel markets in long-haul transport, the performance of the processes evaluated herein to produce renewable diesel were considerably more costly and had weaker environmental performance compared to ethanol made from biomass sorghum. Low process yields were the cause of low environmental and economic performance. However, improving process yields is necessary but not sufficient to achieve a competitive fuel cost. Reductions in capital cost (through technological advances in the electrochemical reactor) and modifying the microorganism to improve FFA yield from the sugars (higher theoretical yields) should be studied to improve the economic viability of the renewable diesel. Finally, our LCA findings show a need to reduce chemical and nutrient inputs and to improve process yields in order to meet U.S. policy objectives.

Author contributions

S.S. and V.L. conceived the work. V.L. completed the Aspen Plus simulations, techno-economic analysis calculations and life cycle assessment. V.L. wrote the original draft. V.L. and S.S. wrote, reviewed and edited the manuscript. M.B, K.Y.S., P.V.V, J.M, S.E. and M.K. contributed experimental data and reviewed the manuscript. S.S. supervised the work.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

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