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Life Cycle Assessment of Bioethanol Production: A Case Study from Poplar Biomass Growth in the U.S. Pacific Northwest

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Abstract: Biomass appears to be one of the most prominent renewable resources for biofuels such as bioethanol, mainly due to its better environmental performance compared with fossil fuels. This study addresses a comprehensive environmental performance of bioethanol production, employing empirical data from hybrid poplar grown in the U.S. The study considers 1 MJ as a functional unit and employs a cradle-to-grave approach, which entails the feedstock and harvesting production of poplar, transport to a biorefinery, bioconversion of the biomass process, and fuel use. On average, bioconversion is the main contributor to environmental degradation in all the categories evaluated (77%). The second main contributor is either the feedstock and harvesting production of poplar (17%) or fuel use (6%), depending on the environmental category. Thus, focusing on only one category may induce a misinterpretation of the environmental performance of bioethanol production. Finally, environmental credits in the global warming potential (GWP) category were obtained from the carbon sequestered in the biomass during the growing period and from avoided fossil fuel emissions due to electricity production from a renewable source. This means that the net GWP of the life cycle of bioethanol from poplar biomass is slightly negative (-1.05×10^{-3} kg CO_2-eq·MJ^{-1}).

Keywords: LCA; bioethanol; carbon sequestration; bioconversion process; global warming potential

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1. Introduction

Fossil fuels are one of the major environmental concerns because of, among other factors, greenhouse gas (GHG) emissions that result in climate change [1]. Different renewable resources (e.g., solar, wind, geothermal, and biomass) have been explored as fossil fuel alternatives to mitigate the environmental impact [2]. Biomass is one of the world's main sources of energy and is among the most available feedstocks [3]. Non-woody biomass comprises organic materials from a wide range of agricultural processes, animal waste, and herbaceous plants [4]. Woody biomass includes native forest biomass, woody waste, forest residues, and short rotation forestry [5]. Particularly, short rotation woody crops (SRWCs), such as poplar, are an ideal biomass because they are high-yielding, require few inputs, and could be grown on a rotation of 3 to 4 years [6,7]. In fact, Morales-Vera et al. [8] identified that the SRWC of poplar presents an attractive option for diversifying and expanding biomass for biofuel production, which, in addition, increased rapidly for a compound global annual growth rate of 7.6% from 2016 to 2022 [9]. These characteristics make woody biomass from SRWCs of special interest as a source of renewable energy.

Biofuels, such as bioethanol and biogas, come from biomass [10]; bioethanol, in particular, is a potential candidate to replace a portion of fossil fuels [11]. Worldwide bioethanol production has experienced a continuous increase due to the mandates introduced in different countries to replace fossil fuels to mitigate climate change and secure energy availability [12]. In 2019, production was reported to be 29 billion gallons, of which the United States (U.S.) and Brazil were the main producers at 58 and 28%, respectively, followed by the European Union at 5% [13]. In addition, demand is expected to increase due to the unprecedented consumption patterns [10].

In the case of the U.S., ethanol production moved from 2007 million gallons per year in 2000 to 17,436 million gallons in 2019 [14]. Moreover, it is expected that biofuels from woody biomass will displace 30% of the petroleum consumed by 2030 [15]. The market for bioethanol in the U.S. is based on the feedstock, type of vehicle, and geographical area [9]. Focusing on the feedstock, woody biomass constitutes 6% of total U.S. bioethanol [9]. The Pacific Northwest states of Oregon, Washington, and Idaho represent, on average, 0.5% of the national bioethanol production. In particular, Oregon's clean fuels program recently included bioethanol to help reduce the carbon intensity from transport [16]. Moreover, the hybrid poplar in this region is one of the most promising purpose-grown energy crops; it presents rapid growth, requires a minimal amount of agrochemicals, regenerates by coppice, and has high biomass productivity [8,17].

The environmental analysis of biofuels such as bioethanol is critical for the sustainable production and the development of technology and policies [18]. In recent decades, the environmental performance of products and services has been assessed mainly using life cycle assessment (LCA), a quantitative methodology that assesses the potential environmental impacts of products and services over their life cycle. This is achieved by quantifying the emissions and discharges that could affect the environment, such as global warming potential, acidification, and eutrophication [19]. Thus, the LCA is commonly accepted for assessing the environmental effects of bioethanol production [20]

Several works have analyzed the environmental performance of bioproducts such as itaconic acid [21], polylactic acid [22], and biochar [23]. In the case of bioethanol fuel, some studies have noted improved environmental performance in GHG emissions compared to emissions from fossil fuels [24–26]. GHG emissions from the bioethanol life cycle have been widely addressed in different contexts [27–29]; however, analysis of these emissions is still a subject of debate since system boundaries vary among different researchers, which affects calculations [30]. Furthermore, focusing only on GHG emissions rather than a full environmental performance could lead to the misinterpretation of environmental performance. In fact, as mentioned by Morales et al. [11], although the comparison of GHG emissions to energy balance between bioethanol and fossil fuels has been widely addressed, the same cannot be said for other environmental categories such as acidification and eutrophication potentials. In addition, most studies that evaluate the environmental impacts of bioethanol production use previously published data; thus, they do not include experimental values for biomass production or conversion, which means that bioethanol production under this biorefinery context is not analyzed. Consequently, this research intends to provide a comprehensive life cycle assessment of bioethanol production using empirical field data and covering a wide range of potential environmental impacts.

Based on the abovementioned, the aim of this study is to analyze the environmental performance of bioethanol production from hybrid poplar grown in the Pacific Northwest of the U.S. The analysis was conducted by means of an LCA methodology using experimental data, process simulation in AspenPlus™ (Aspen Technology, Inc., Bedford, MA, USA), and a literature review. In addition, a comparison with other U.S. SRWCs and conventional gasoline was made.

2. Materials and Methods

2.1. Goal and Scope Definition

In this study, the LCA methodology was used to analyze the environmental performance of bioethanol production and its combustion in a dedicated car. As such, this study followed the ISO 14,040 [31] and 14,044 guidelines [19]. Bioethanol production comes from poplar biomass over 21 years, while its use as a fuel is analyzed in an automobile. In this sense, this study comprises all stages of the bioethanol life cycle from site establishment for poplar production to combustion. The life cycle stages were biomass production and harvesting (including C sequestration processes), transport to biorefinery, bioconversion of the biomass process (including ancillary chemicals and avoided electricity production), and fuel use. This approach is called the cradle-to-grave system boundary. Figure 1 presents the system boundaries considered in this study. In addition, a functional unit (FU) that properly reflects the product or process being studied in a quantitative manner needed to be established [19]. Therefore, the selected FU was 1 mega joule (MJ), a common FU in biofuel LCAs since it allows for a comparison among different types of fuels in relation to their energy potential [11].

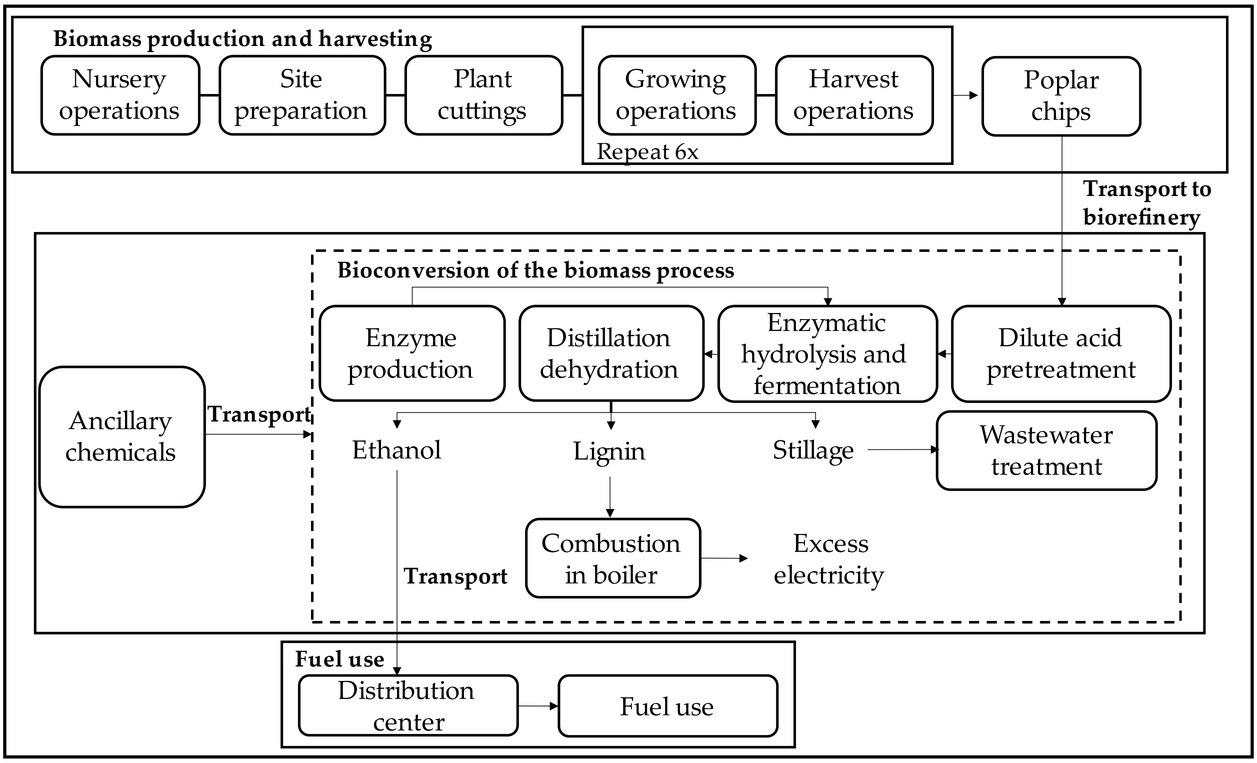


Figure 1. System boundaries of bioethanol production from a hybrid poplar.

2.2. Life Cycle Inventory

As mentioned before, this study comprises the stages of feedstock and harvesting production of poplar, transport to biorefinery, bioconversion of the biomass process, and fuel use. Consequently, this section presents the life cycle inventory (LCI) for each stage.

2.2.1. Feedstock and Harvesting Production

The LCI of poplar for feedstock production and the harvesting stage was obtained from operational data provided by "GreenWood Resources Inc." (Portland, OR, USA) from an experimental site in Jefferson, OR. The poplar is a hybrid of *Populus trichocarpa* and *Populus deltoids*, and production was conducted in cycles of tree years for each. The first three years of feedstock production included growth in a nursery and preparing the planting location for transplanting the following year [32]. Nursery operations included the application of herbicides and insecticides. While an insecticide was used only in the first year of the nursery stage, an herbicide was used throughout the whole period each year. Once they are large enough, the trees are turned into cuttings and transported to cold storage. Preparing the planting location for the cuttings depended on site-specific characteristics, but, in general, the land underwent heavy and finished disking, smoothing, row marking, and herbicide application. The cuttings were planted the following year and grew for two years before the first coppicing, which promoted the growth of multiple stems per stump. Following the first coppicing, the trees were harvested every 3 years for six cycles. The trees were harvested by a forage harvester. No storage of the poplar biomass was needed at the tree farm or biorefinery as the trees were harvested year-round, following a just-in-time harvest management scheme.

This stage also considers the sequestration of carbon during the growing of biomass. Consequently, biogenic CO_2 was also accounted for in the full carbon mass balance. The biogenic CO_2 is the carbon that is part of the natural carbon cycle, which comprises CO_2 sequestrated by the poplar biomass and the CO_2 produced from the biomass combustion. Even though non-biogenic CO_2 includes CO_2 emissions from fossil fuel combustion, it was included in the analysis. This study accounted for both types, which were reported separately following ISO guidelines [19]. Table 1 presents the main inputs used at the feedstock and harvesting production stage. A detailed LCI is found in Table S1 in the Supplementary Materials.

Table 1. LCI of the feedstock and harvesting production stage.

Material	Unit	Average Annual Amount
Forest Annual Carbon Uptake	Tons $C{\cdot}ha^{-1}{\cdot}yr^{-1}$	7
Bioenergy Removals		
Dry Tons of Dedicated Harvest	Dry $ton{\cdot}ha^{-1}$	15
Hardwood Uncollected Biomass	Dry $ton{\cdot}ha^{-1}$	1
Energy Use		
Diesel	$BTU{\cdot}ha^{-1}$	3,590,012
Lubricant	$BTU{\cdot}ha^{-1}$	64,129
Pesticide Use		
Herbicide	$g{\cdot}ha^{-1}$	5239
Insecticide	$g{\cdot}ha^{-1}$	1

2.2.2. Transport to Biorefinery

The harvested poplar trees were towed alongside the harvest in forage wagons to collect the chips, which were then loaded into a chip van by a silage blower to be transported to the biorefinery. It was assumed that the chips needed to be transported over an average distance of 100 km. This distance was selected based on a likely maximum economic transport distance proposed by [33]. Finally, it was assumed that chip vans would return empty to the poplar tree farm.

2.2.3. Bioconversion of the Biomass Process

Similar to the NREL corn-stover-to-ethanol model [34], the bioconversion of the biomass to ethanol was modeled using AspenPlus™, a chemical engineering software using an NRTL base property. All major units and reactions were modeled with an RStoic block, and literature values were used for operating temperature, pressure, and fractional conversion data. Pretreatment and fermentation yields as well as conversion factors were conservative estimates in collaboration with our laboratory. Distillation columns were modeled with rigorous vapor–liquid equilibrium calculations in Aspen using the RADFRAC model (Aspen Technology, Inc., Bedford, MA, USA). Consequently, the NREL corn-stover-to-ethanol model [34] was modified using laboratory-based data and literature to yield 282 L of ethanol per ton of poplar feedstock. Poplar chemical composition was 38.5% glucan, 14.3% xylan, 0.5% arabinan, 0.7% galactan, 1.8% manan, 24.2% lignin, 1.3% ash, 4.4% acetate, and 14.3% extractives. The biorefinery processes included 2.1% diluted acid pretreatment of the chips at 195 °C. After pretreatment, the hydrolysate slurry was raised to 5–6 pH using ammonia. The temperature of the saccharification was 48 °C using a cellulase loading of 20 mg enzyme protein/g cellulose to achieve 90% conversion of cellulose to glucose. Fermentation was carried out at 32 °C using *Zymomonas Mobilis* bacteria, achieving 95 and 85% of conversion to ethanol for glucose and xylose, respectively. Enzymes were produced on site by *Trichoderma reesei*, using corn syrup as the primary carbon source. Ethanol recovery was achieved by distillation of a nearly azeotropic mixture with water and then purified to 99.5% using vapor-phase molecular sieve adsorption. The solids from the distillation and wastewater treatment and the biogas from anaerobic digestion were combusted to produce high-pressure steam to produce electricity and process heat. All necessary chemicals, transportation (66 km), and processes required by each bioconversion process were included in the LCAs. Table 2 depicts the inventory of the bioconversion of the biomass process stage. Amounts are normalized for the production of 1 MJ of bioethanol.

Table 2. LCI of the bioconversion of the biomass process stage to produce 1 MJ of bioethanol.

Inputs	Unit	Amount
Poplar chips (bone dry)	g	170.53
Sulfuric Acid (93%)	g	4.05
Lime	g	1.62
Ammonia	g	3.52
Corn steep liquor	g	2.67
Sodium hydroxide (50%)	g	14.00
Diammonium Phosphate	g	0.25
Sulfur Dioxide	g	0.03
Outputs (conversion process)		
Carbon dioxide	g	236.07
Carbon monoxide	g	0.03
Nitrogen oxides	g	0.03
Sulfuric dioxide	g	0.12
Bioethanol	MJ	1
Excess Electricity (avoided production)	kW	0.036

In this stage, avoided electricity production was also considered. To perform this, a system expansion was considered for bioethanol by-products as fuel to generate electricity [19], following ISO guidelines. This approach was chosen for two main reasons. First, as stated in [35], "electricity is currently produced from other sources and life cycle data for the production of electricity from these other sources can be obtained". Second, the expansion is one of the most common methods used in biofuel LCAs to deal with by-products [36]. In this context, it was assumed that the electricity would be sold to the grid, thereby displacing electricity produced from natural gas and obtaining credit for displacing a fossil fuel.

2.2.4. Fuel Use

Finally, the bioethanol produced is assumed to be combusted in a dedicated ethanol automobile using 100% ethanol (E100). For this, bioethanol was transported to a distribution center using distances estimated based on [37]: 66 km by truck, 372 km by rail, and 975 km by water. The emissions produced from combustion were modeled using GREET software [38].

2.3. Life Cycle Assessment

The LCA was conducted using the TRACI 2.1 life cycle impact assessment method that evaluates 10 categories: global warming potential (GWP) (kg CO_2-eq), eutrophication (kg N eq), acidification (kg SO_2 eq), ozone depletion (kg CFC-11 eq), smog (kg O_3 eq), carcinogenics (CTUh), non carcinogenics (CTUh), respiratory effects (kg $PM_{2.5}$ eq), ecotoxicity (CTUe), and fossil fuel depletion (MJ surplus). The LCA was modeled in SimaPro v.7.3.0 software [39], using mainly the U.S. LCI database [40]. When no appropriate data were available, the Ecoinvent database was also used [41]. Biochemical conversion was modeled using Aspen Plus [42].

2.4. Uncertainty Analysis

Uncertainty analysis in this work was required to analyze the impact of original data uncertainty on the stability of the results. Traditional sensitivity analysis (one factor at a time) might not represent real-life scenarios where more than one independent parameter varies simultaneously. Therefore, traditional sensitivity analysis and a Monte Carlo simulation were conducted to analyze the impact of key parameters of the biochemical conversion model of poplar to ethanol. The model parameters included in the analysis are the enzymatic hydrolysis and fermentation yields and the glucan content (dry basis) (Table 3). Variations in these yields (from enzymatic hydrolysis and fermentation) and the glucan content affect the key process indicators (KPIs) of plant ethanol yield, net electricity export to the network, and the plant CO_2 emissions. For instance, a higher glucan content results in a higher yield of ethanol per ton of feedstock [43], a reduction in lignin that influences the production of electricity in the biorefinery, which directly affects the system's CO_2 emissions. Thus, the aim of the sensitivity analysis was to calculate a local effect (or sensitivity) of a 1% variation in each parameter—changed one at a time—over the selected KPIs around the base case values. On the other hand, the Monte Carlo analysis provides a more global view of the effects over the KPIs of changing the model parameters simultaneously and over a wider range (see Table 3). Thus, the information gathered from the 5000 scenarios was used to assess the likelihood of achieving the KPI values used in the base case.

Table 3. Triangular distribution parameters for random variables used in the Monte Carlo analysis.

Parameter	Minimum	Base Case	Maximum
Glucan-to-glucose yield in enzymatic hydrolysis	0.70	0.90	0.95
Glucose-to-ethanol yield in fermentation	0.75	0.95	0.97
Glucan content in poplar (wt. fraction, dry basis)	0.350	0.385	0.465

A surrogate modeling approach was selected [44] to calculate the outputs from the uncertainty analysis because of the large number of scenarios (5000) in the simulation. The number was selected to produce a reasonable coverage of the three-dimensional space of the variables in the analysis: enzymatic hydrolysis, glucose fermentation yields and dry glucan content. In this approach, instead of solving a complete Aspen Plus simulation, in each scenario, a surrogated representation of the Aspen Plus flowsheet was solved. The surrogated model was built using mass and energy balance relationships and chemical and thermophysical data from the 2011 NREL report on the biochemical conversion of lignocellulosic biomass to ethanol [34]. The surrogate model includes the same unit operations and stages as the 2011 NREL model. Other design considerations and simplifications can be found in Scott et al. [44].

The surrogate model was used to perform a Monte Carlo analysis to calculate the ethanol yield in liters per metric ton of dry poplar biomass, net electricity production (plant electricity production minus plant consumption), and specific CO_2 production (kg of CO_2 emitted per liter of ethanol produced), including emissions from the fermentation and distillation scrubbers, aerobic lagoons in wastewater treatment, and emissions from burning (including the CO_2 in the combusted biogas). Each of the 5000 scenarios represents a realization of the three random parameters (enzymatic hydrolysis yield, glucose fermentation yield, and glucan content) sampled from the three triangular distributions defined in Table 3. The lignin mass fraction was calculated as the balance between xylan, extractives, and glucan mass fraction.

The surrogate model contained 2011 continuous variables and 952 linear constraints and 459 nonlinear constraints. To conduct the analysis, the non-linear solver CONOPT 3 was employed in the GAMS v.27.3 software [45].

3. Results

3.1. Life Cycle Assessment of Bioethanol from Hybrid Poplar

Table 4 shows the contribution of the life cycle stages of bioethanol production from hybrid poplar biomass. According to this table, four main activities generate environmental impacts (i.e., feedstock and harvesting production, transport to biorefinery, bioconversion of the biomass process, and fuel use). However, two sources of environmental credits as carbon in biomass and avoided electricity production were estimated.

Table 4. Environmental impacts of each life cycle stage of bioethanol production.

Environmental Impact Category	Feedstock and Harvesting Production	Transport to Biorefinery	Bioconversion of the Biomass Process	Fuel Use	Carbon in Biomass	Avoided Electricity Production	Total Net Value
Global warming potential (kg CO_2 eq)	2.6×10^{-2}	3.9×10^{-5}	2.4×10^{-1}	6.7×10^{-2}	-3.1×10^{-1}	-2.3×10^{-2}	-1.1×10^{-3}
Eutrophication (kg N eq)	4.2×10^{-6}	4.4×10^{-8}	9.4×10^{-6}	1.1×10^{-6}	–	-1.6×10^{-6}	1.3×10^{-5}
Acidification (kg SO_2 eq)	3.6×10^{-5}	8.1×10^{-7}	3.6×10^{-4}	1.7×10^{-5}	–	-2.0×10^{-4}	2.1×10^{-4}
Ozone depletion (kg CFC-11 eq)	6.8×10^{-11}	1.5×10^{-15}	2.1×10^{-9}	–	–	-1.6×10^{-11}	2.2×10^{-9}
Smog (kg O_3 eq)	1.1×10^{-3}	2.4×10^{-5}	1.8×10^{-3}	7.0×10^{-4}	–	-3.2×10^{-4}	3.4×10^{-3}
Carcinogenics (CTUh)	4.6×10^{-11}	5.3×10^{-13}	1.6×10^{-10}	–	–	-9.6×10^{-11}	1.1×10^{-10}
Non carcinogenics (CTUh)	4.0×10^{-10}	5.1×10^{-12}	7.3×10^{-9}	–	–	-1.2×10^{-9}	6.6×10^{-9}
Respiratory effects (kg $PM_{2.5}$ eq)	8.3×10^{-7}	1.3×10^{-8}	2.1×10^{-5}	1.7×10^{-6}	–	-1.2×10^{-5}	1.1×10^{-5}
Ecotoxicity (CTUe)	7.4×10^{-3}	9.8×10^{-5}	9.9×10^{-3}	–	–	-1.5×10^{-2}	2.0×10^{-3}
Fossil fuel depletion (MJ surplus)	5.5×10^{-3}	7.0×10^{-5}	3.3×10^{-2}	–	–	-5.3×10^{-2}	-1.4×10^{-2}

Regarding the activities that generate environmental impacts, as presented in Figure 2, bioconversion of the biomass process had a significant impact on all categories, from 50% (smog) to 97% (ozone depletion potential), for an average of 77%. Feedstock and harvesting production was the second contributor in eight of ten categories, with a mean value of 17%, ranging from 3% (ozone depletion) to 42% (ecotoxicity). In the remaining two categories (GWP and respiratory effects), the second main contributor was fuel use, with a mean value of 6%. The stage of transport to biorefinery represented less than 1%, on average, in all environmental impact categories.

Concerning the environmental credits, the contribution of each source to the net value depends on the category evaluated. In GWP, carbon in biomass and avoided electricity production were identified, while in the remaining categories, only avoided electricity production generated environmental credits. This is because carbon in biomass refers to the amount of C captured during the photosynthesis process, being comparable in terms of CO_2 eq, while avoided electricity production refers to the electricity that is sold to the grid, displacing electricity produced from natural gas, obtaining credit for displacing a fossil fuel, and therefore decreasing environmental impacts in all categories.

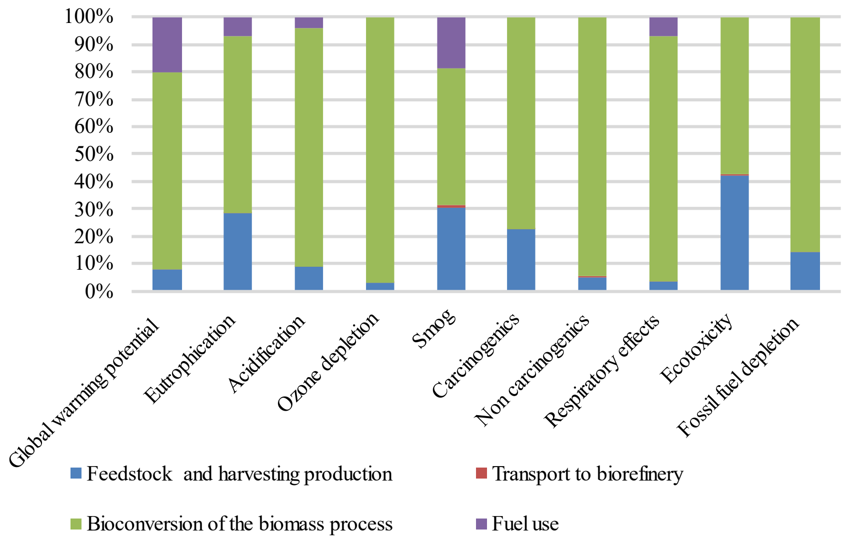


Figure 2. Mean contribution of each stage to the environmental impacts of bioethanol production.

When the focus is on the net value of each category (measured as the sum of environmental impacts and environmental credits), some findings can be highlighted. The environmental credits of CO_2 eq are -3.3×10^{-1} kg CO_2 eq (see Table 4). From this, the carbon stored in the biomass during the growth period represented 93% of the total offset, while avoided electricity resulted in a GWP credit of 7%. Thus, the net GWP obtained was -1.05×10^{-3} kg CO_2-eq·MJ^{-1}. This means that the net GWP of the life cycle of bioethanol from poplar biomass was slightly negative, since carbon emissions from ethanol production and use were similar to the carbon absorbed during the period growth and the avoided fossil fuel emissions due to electricity produced from a renewable source. For the fossil fuel depletion category, environmental credits (-5.3×10^{-2}) are also higher than the environmental impacts (3.9×10^{-2}). This means that the net fossil fuel depletion of the life cycle of bioethanol from poplar biomass was also slightly negative. This could be explained by electricity generated during bioethanol production avoiding the production of electricity from non-renewable sources such as natural gas. For all other categories, the impacts are higher than the credits, and consequently, the net impacts are positive.

3.2. Uncertainty Analysis

Agreement between the Aspen Plus simulations and the surrogate model used in the Monte Carlo analysis was verified by comparing the analyzed variables one at a time for extreme instances of parameter values—-the maximum and minimum values and the base case in Table 3. The largest difference between both models was less than 2% for the variables under analysis; thus, the agreement between the models was deemed satisfactory.

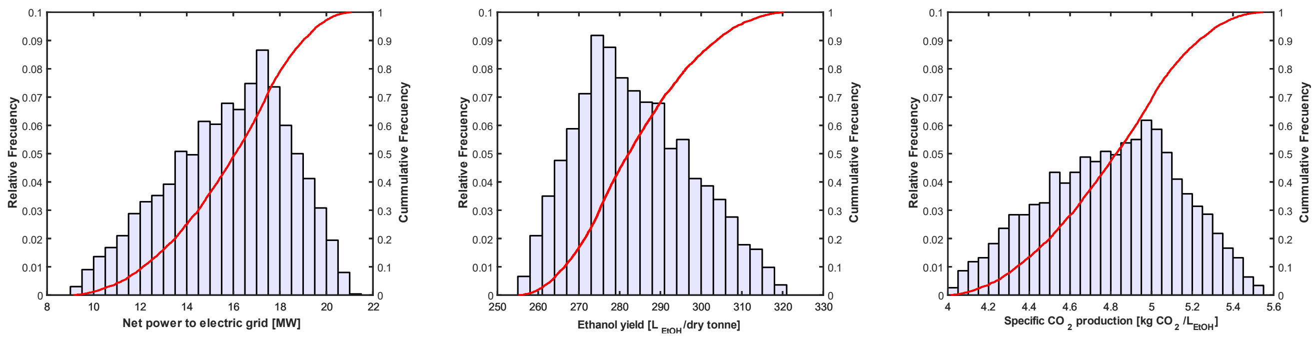
Table 5 summarizes the results of the traditional sensitivity analysis. Sensitivities were calculated from one-at-a-time variations in the independent variables: glucan content, glucose-to-ethanol yield, and glucan-to-glucose yield, within the intervals shown in Table 3. The values in Table 5 correspond to the percent change in ethanol yield, the net electricity production (plant electricity production minus plant consumption), and the specific CO_2 production after a 1% variation in the independent variables. These sensitivities were calculated assuming a linear relation between the independent and dependent variables; therefore, the Pearson correlation coefficient (r) is also shown. The results indicate that variations in glucan content had the largest sensitivity. Interestingly, the coefficient indicated that, when the plant ethanol yield increased, net exported power and CO_2 emissions were reduced. Similar results were found in the technoeconomic analysis of ethanol production from corn stover [46].

Table 5. Percent change in the plant ethanol yield, net power exported to the grid, and CO_2 emissions from a 1% change in the glucan-to-glucose yield, glucose-to-ethanol yield, and glucan content. A linear relationship was assumed; therefore, the Pearson coefficient is also presented.

	Plant Ethanol Yield		Net Exported Power		CO_2 Emissions	
	Percent Change	r	Percent Change	r	Percent Change	r
Glucan-to-glucose yield in enzymatic hydrolysis	0.80	0.98	−1.46	−1.00	−1.02	−1.00
Glucose-to-ethanol yield in fermentation	0.84	1.00	−1.41	−1.00	−1.07	−1.00
Glucan content in poplar (wt. fraction, dry basis)	5.37	0.98	−3.22	−0.98	−2.02	−0.98

Figure 2 presents the results from the Monte Carlo simulation as cumulative and relative frequency distributions conducted using 5000 scenarios (see Table 3) and combining triangular distributions.

According to Figure 3, different probabilities of achieving or exceeding the base case scenario values were obtained when triangular distributions of the random parameters were used. For net electricity production, the probability of achieving or exceeding the base case scenario (17.8 MW) was 23.8%. For the base case scenario, ethanol yield (275 L·ton of $EtOH^{-1}$) was 70.1%. Finally, for the base case scenario, CO_2 production (5.0 kg CO_2 L of $EtOH^{-1}$) was 69.2%. Therefore, even under the wide ranges of model parameters shown in Table 3, there is a 70% chance of having lower specific CO_2 emissions than the ones used in the base case, providing confidence in the results shown in Figure 2 for the net CO_2 emissions.



(**a**) (**b**) (**c**)

Figure 3. Uncertainty analysis results for the net power exported to the electrical grid (**a**), bioethanol yield (**b**), and specific CO_2 production (**c**) using Monte Carlo simulation with 5000 scenarios. Red lines represent the cumulative frequency, while bars represent the relative frequency.

4. Discussion

As mentioned in the Introduction, most studies evaluating the environmental impact of the bioethanol life cycle have focused on the GWP category. This study went further to analyze 10 environmental impacts using empirical data from a hybrid U.S. poplar biomass, the main producer of bioethanol worldwide. As observed in Section 3, the bioconversion of biomass was the main contributor to environmental damage in all categories. This was similar to the study of Budsberg et al. [47], where the biorefinery stage was also identified as the main contributor to the LCA. This could have been due mainly to the ancillary chemicals employed at that stage. In fact, when the bioconversion of biomass is split into ancillary chemicals and the conversion processes, the first ones contribute 74%, on average, in all categories. This was more evident in the category of fossil fuel use, where it contributed 99.9%, which could have occurred since most of the fossil fuel used for bioethanol production was generated for the ancillary chemicals' production.

The stages of fuel use and of feedstock and harvesting production were also identified as important contributors to the environmental impacts. However, their relative contribution depended on the category evaluated. For instance, for GWP, fuel use was the second-largest contributor (after bioconversion of biomass process). This was due to carbon monoxide, carbon dioxide, and nitrogen oxide emissions. In the categories of eutrophication, smog, carcinogenics, and ecotoxicity, feedstock and harvesting production was the second-largest contributor. This could be explained by the use of fossil fuels for agricultural machinery and the use of agrochemicals. This difference in the relative contribution of each stage revealed the importance of conducting an extended LCA rather than focusing only on one category, as mentioned by Morales et al. [11].

The GWP is one of the most analyzed environmental categories of bioethanol production from a woody biomass [11]. In this sense, a comparison of GWP with two additional SRWCs grown in the U.S. and with gasoline obtained from the results of Lippke et al. [32] was carried out in this study. In particular, the GWP of the life cycle of bioethanol production from willow, eucalyptus, and gasoline were compared with the results from our study. Figure 4 presents the GWPs from this study and those reported by Lippke et al. for willow, eucalyptus, and conventional gasoline [32]. In addition, it also depicts the net GWP for gasoline and each SRWC. Comparing the GWP of the three SRWCs, even though poplar presented the higher GWP compared with willow and eucalyptus, it also presented the highest amount of sequestered carbon during biomass growth: 312 g C, willow 264 g C, and eucalyptus 268 g C. This resulted in a slightly negative net GWP value for eucalyptus (-4.68 g CO_2-eq·MJ^{-1}) and hybrid poplar (-1.05 g CO_2-eq·MJ^{-1}), while willow presented a positive net value: 26.96 g CO_2-eq·MJ^{-1}. This can be explained by poplar trees being able to sequester a higher amount of carbon than willow or eucalyptus during the growth stage. For instance, Rytter (2012) [48] reported the total woody biomass of willow sequestration as 3.49 mg C·ha^{-1}·yr^{-1} and poplar sequestration as 4.01 mg C·ha^{-1}·yr^{-1}. Furthermore, a small GWP credit was generated from avoiding the production of marginal electricity production for all SRWCs. In this sense, carbon emissions from the bioethanol life cycle are balanced by carbon sequestration during the growth phase for willow and poplar and the displacement of fossil fuel-produced electricity by renewable electricity produced in the bioconversion process.

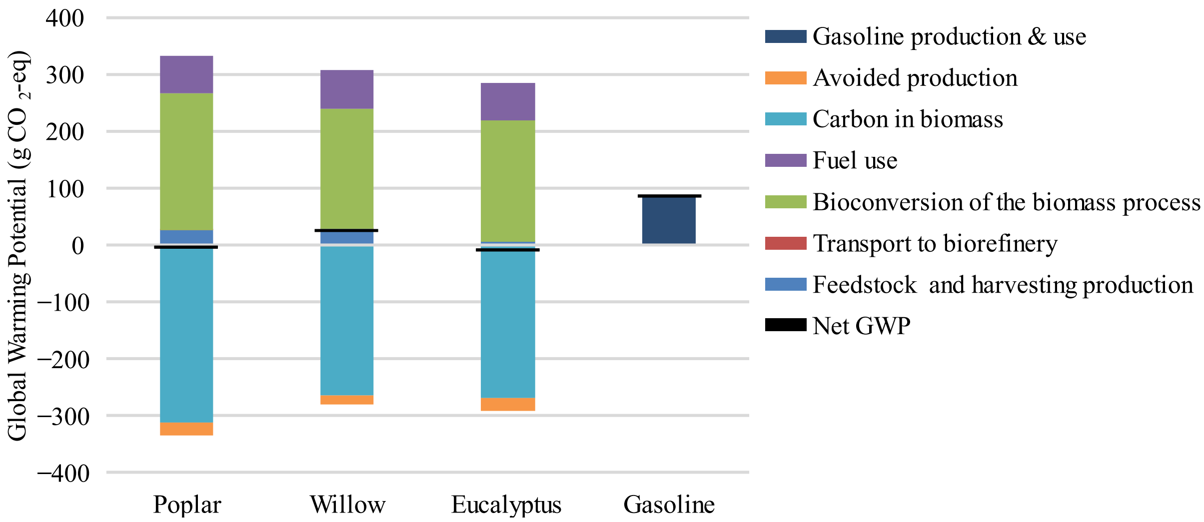


Figure 4. Comparison of the GWP of poplar in this study with the GWP of willow, eucalyptus, and gasoline extracted from [29]. The black line represents the net GWP for each fuel.

Considering the GWP from the bioethanol of poplar and gasoline, there was a notable increase when shifting from poplar bioethanol to gasoline. The net GWP of bioethanol from poplar was -1.05 g CO_2-eq·MJ^{-1}, while for gasoline it was 88 g CO_2-eq·MJ^{-1}. This difference was highly influenced by the carbon sequestered during crop growth, which contributed to offsetting GHG emissions [49]. In fact, a literature review conducted by Wiloso et al. revealed that most of the studies found lower GHG net emissions of bioethanol compared to gasoline [33]. However, in other environmental categories, such as acidification and eutrophication, the effect from gasoline was lower. For instance, the acidification potential of bioethanol from poplar was 99% higher than the values for gasoline reported in [49,50], and the eutrophication potential was 100% higher than the values reported in [50]. These are in line with the findings of Wiloso et al., who stated: "studies based on a more complete set of impact categories such as eutrophication, acidification and toxicity are likely to lead to different outcomes, particularly when productive land or coal is included in the bioethanol system" [33].

Comparing the environmental profile of the bioethanol production in this study with those reported in the literature, some differences can be highlighted. For instance, in 2012, Gonzalez-García et al. reported a net GWP of -0.619 kg CO_2-eq·kg of ethanol^{-1} [51]. Using the energy density of 29.6 MJ·kg^{-1} reported by Lippke et al. [32], the GWP of Gonzalez-García et al. was -0.021 kg CO_2-eq·MJ^{-1}. This higher net GWP with respect to the results from our study could be the result of considering the subsystems of SRWC cultivation and ethanol production up to the biorefinery stage, while our study also considered transport to the biorefinery and the use of a dedicated car (E100). However, Gonzalez-García et al. reported a higher value of acidification (1.7 g SO_2-eq·MJ^{-1}) compared with our result (0.2 g SO_2-eq·MJ^{-1}) because of ammonia (NH_3) emissions from nitrogen-based fertilizers [51]. Poplar cultivation in our study did not consider fertilizer application, which could explain the lower value. In 2010, Gonzalez-García et al. addressed an environmental profile of poplar biomass ethanol as a transport fuel in Southern Europe and obtained lower values in ozone depletion (6.8×10^{-10} kg CFC-11 eq·MJ^{-1}) compared to our study (2.2×10^{-9} kg CFC-11 eq·MJ^{-1}) [49]. However, their values for the GWP and acidification were higher by 132% and 6%, respectively, mainly due to the use of fertilizers during the feedstock stage.

Finally, concerning the uncertainty analysis using Monte Carlo simulation for the three output variables (net electricity production, ethanol yield, and CO_2 production), it was interesting to observe that, while ethanol yield and CO_2 production resulted in similar probabilities for achieving or exceeding the base case scenario, net electricity production had a lower value.

The use of Monte Carlo methods in techno-economic analyses of lignocellulosic feedstocks for fuels has been used to model the effects of multiple simultaneous price changes [52]. However, uncertainty in model parameters has seldom been explored. The reason behind this trend is that prices only affect the economic model; therefore, uncertainty can be propagated easily without recalculating the mass and energy balances. In this work, instead of fully propagating the uncertainty through the Aspen Plus and then the LCA model, a surrogate approach was adopted to calculate the probability of achieving key performance indicator values above those defining the base case used in the LCA. Figure 3 indicates that electricity exports to the grid are likely to be lower than those assumed in the base case, leading to a reduction in emissions avoided and thus to an increase in the global warming potential. A similar result was previously reported by Spatari et al. [46], who found that surplus electricity exports play an important role in the total GHG emissions of different lignocellulosic-to-ethanol production processes.

5. Conclusions

In this study, a comprehensive life cycle assessment of bioethanol production from a short rotation woody crop of poplar grown in the U.S. was conducted using empirical data. The study covered the stages of feedstock and harvesting production of poplar, transport to biorefinery, bioconversion of the biomass, and fuel use in a dedicated car (E100), using 1 MJ as a functional unit. A total of 10 environmental categories were evaluated using the TRACI 2.1 life cycle impact assessment method performed in the SimaPro v.7.3.0 software.

The results reveal that biomass bioconversion was the main contributor in all environmental categories, mostly due to the ancillary chemicals employed, followed in eight categories by the stage of feedstock and harvesting production, and in two categories, by fuel use. This difference in the contribution of each stage showed the importance of conducting an extended LCA, rather than focusing only on one category.

Focusing on the GWP category, the net value of the whole life cycle of bioethanol is slightly negative since carbon emissions are similar to the carbon absorbed and avoided. In addition, when comparing the GWP of bioethanol production obtained in this study with those obtained for eucalyptus and willow SRWCs in the literature, bioethanol from hybrid poplar and eucalyptus demonstrated better environmental performance, because their net GWP value were slightly negative (-1.05 and -4.68 g CO_2-eq·MJ^{-1}, respectively), even though it is important to mention that the literature shows that poplar has a better ability to sequester carbon.

Finally, future research might explore additional approaches to assess both environmental and cost ethanol life cycles to find new opportunities to improve the sustainability of ethanol production. Furthermore, since the bioconversion of biomass process is an important contributor to all categories, future studies could focus on additional environmentally safe ways to produce ethanol in a biorefinery.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/fermentation8120734/s1, Table S1: Life cycle inventory of the feedstock and harvesting production.

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