1	Environmental and economic analysis of bioethanol production from sugarcane molasses
2	and agave juice
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15	Abstract
16	In this article, sugarcane molasses and agave juice were compared as potential feedstocks for
17	producing bioethanol in Mexico in terms of their environmental impact and economic factors. Life
18	cycle assessment (LCA) using SimaPro was carried out to calculate environmental impacts by
19	using a cradle-to-gate approach. A preliminary economic analysis was performed to determine the
20	economic feasibility of the studied options. Also, capital goods costs were obtained using the
21	Aspen Plus economy package. Moreover, a sensitivity analysis was involved to compare the
22	environmental and economic viability of producing bioethanol from sugarcane molasses and agave

23 juice. LCA results revealed that cultivation and fermentation were the most harmful stages when 24 producing bioethanol from sugarcane molasses and agave juice, respectively. Furthermore, when it was derived from agave juice rather than sugarcane molasses, it had more environmental 25 26 benefits. This was ascribed to the lower consumption rate of fertilizers, pesticides, and emissions 27 given off from the former. Regarding financial aspects, the preliminary analysis showed that producing bioethanol was not economically viable when grid energy alone was used. However, if 28 29 power from the grid is partially replaced with renewable energy, producing bioethanol becomes 30 economically feasible, and sugarcane molasses is the most suitable feedstock.

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32 Keywords: Bioethanol, Sugarcane bagasse, Agave bagasse, Life cycle assessment, Economic
 33 analysis

34 **1. Introduction**

35 Undoubtedly, climate change - mainly due to the increase in CO₂ emissions from fossil 36 fuel combustion, industry, and transport - is a severe threat to life on our planet. For instance, about 3% of greenhouse gases (GHG) emissions are associated with transport 37 38 (Oliver et al. 2017). Therefore, renewable energy poses an alternative for tackling these 39 adverse effects (Sanchez et al. 2020b). Mexico, whose main source of energy is crude oil, 40 is considered to be one of the largest contributors to CO₂ emissions in Latin America 41 (Hanif 2017, Sarmiento et al. 2019). Hence, it is generally agreed that it must change from 42 crude oil to renewable fuels if it is to overcome the unfavorable effects of climate 43 change(Rendon-Sagardi et al. 2014). Bioethanol is one potential renewable fuel, whose 44 combustion is more efficient than gasoline and, consequently, gives off fewer emissions 45 of pollutants such as SOx, NOx and particulate matter (Zabed et al. 2017).

46 Bioethanol is produced from a wide range of materials and can be classified into first, 47 second, and third generation. First generation bioethanol is produced from sugar and 48 starchy feedstocks such as molasses and corn, while second and third generations are 49 obtained from lignocellulosic materials and algae, respectively. Bioethanol production 50 spans the following stages: physical pretreatment (i.e., crushing or chipping), hydrolysis 51 (this is only required when both lignocellulosic and algae materials are employed as 52 feedstock), fermentation, and distillation. For sugar materials, such as molasses, 53 hydrolysis is not required since fermentable sugars, such as sucrose, glucose, and 54 fructose, are freely available for metabolisation by microorganisms during fermentation 55 under anaerobic conditions. Yeasts, such as Saccharomyces cerevisiae, are the most 56 widely used industrially, since they produce a large amount of ethanol and are highly 57 tolerant to ethanol. (Sanchez et al. 2020a, Sanchez et al. 2020c).

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58 Sugarcane and agave are some potential feedstocks that could potentially be used in 59 Mexico to produce bioethanol and mitigate the impacts associated with climate change. 60 For instance, sugarcane (Saccharum officinarum L.) is an essential crop which is 61 primarily used in sugar production. However, it has become fundamental for producing a 62 wide range of goods in the industry. As a result, economic interests in this crop have 63 increased significantly in recent years (Gómez-Merino et al. 2017, Lopez-Bustamante 64 2015). In Mexico, about 57 million tons of sugarcane are produced annually (SAGARPA 65 2018b). In the extraction process, by-products such as bagasse, sugarcane press-mud, and 66 molasses are also yielded (Dias et al. 2015). The latter is a by-product whose sugar content 67 is 50%, which, in turn, is used to yield bio pesticides, pharmaceuticals, cellulose, acids, 68 and bioethanol, amongst other products.

69 Moreover, agave, also known as "maguey", is a native crop from Mexico and about 70 1.8 million tonnes of it are produced annually (SAGARPA 2018b). Nowadays, 71 approximately 200 species are known and they have been classified into three groups: 72 wild, semi-cultivated, and cultivated (Mandujano Bueno et al. 2018, Nava-Cruz et al. 73 2015, Trejo-Salazar et al. 2016). Among these, Agave Salmiana can grow in areas with 74 low rainfall, low temperatures, and poor fertility soils; hence, it is considered to be 75 economically viable. Furthermore, agave juice is well known for its ability to produce 76 bioethanol by fermentation (Corbin et al. 2016, Tauer et al. 2004).

Although production is low in comparison to sugarcane molasses (1.8 million tons vs. 57 million tons), it has an outstanding economic, cultural, and social impact in Mexico(Pérez Hernández et al. 2016). Hence, it could potentially be used as a feedstock for producing bioethanol to mitigate GHG and to act as a driver for economic and social development in Mexico. Moreover, there is no land competition for food since agave 82 grows on semi-arid lands where food crops cannot be cultivated. Additionally, there is 83 still enough unused land where agave can be cultivated. For instance, in Jalisco and 84 Oaxaca there are about 1.7 million and 60,000 hectares available respectively for 85 cultivating agave, but at present it has only taken up 30% of this land (Núñez et al. 2011). 86 In light of this, the environmental and economic benefits of the Mexican biofuel industry 87 obtained from agave by-products were analyzed. This was performed by comparing it 88 with a highly available feedstock such as sugarcane molasses. In order to assess the 89 environmental benefits of agave crops, a life cycle assessment (LCA) was employed. This 90 internationally standardized approach (International Organization is an for 91 Standardization - ISO, i.e. ISO 14040 and ISO 14044) that enables environmental 92 burdens associated with consuming resources and emissions to be assessed as well as the 93 waste released in the chain of production (ISO14040 2006, ISO14044 2006).

94 To date, there are no studies in which the environmental impacts associated with 95 bioethanol from both sugarcane molasses and agave juice are compared. However, 96 several LCA studies on bioethanol yielded from both these raw materials have been 97 published. For instance, Renouf et al. (2013) performed the LCA for ethanol production 98 with different by-products from sugar extraction. They showed that sugarcane juice had 99 the greatest impact on reducing non-renewable energy and global warming potential 100 (GWP). In addition, Silalertruksa et al. (2017) evaluated the environmental impacts from 101 a sugarcane biorefinery, showing that this could be reduced by integrating waste 102 valorization. Papong et al. (2017) studied the environmental benefits of producing 103 bioethanol from cassava and molasses in Thailand, concluding that using it as a transport 104 fuel reduced GHG emissions. However, eutrophication potential (EP) increased as did 105 water consumption potential (WCP) in comparison with gasoline. Furthermore, Yan et

al. (2011) evaluated bioethanol production from *Blue Agave Tequilana Weber*. They
proved that agave was the optimum choice for producing first-generation bioethanol in
comparison to corn, switchgrass, and sugarcane in terms of energy and GHG balances
(Yan et al. 2011).

In short, since both crops were profitable in Mexico, it was deemed beneficial to determine which was most beneficial in terms of the environment and economy. In light of this, the goal of this study was to compare the environmental burdens and economic feasibility of producing bioethanol from sugarcane molasses and agave juice on the basis of these chains of production in Mexico.

115 **2.** Methodology

116 **2.1. Life cycle assessment**

117 **2.1.1. Definition of goal and scope**

A LCA was carried out considering the cradle-to-gate approach, in which the following stages were evaluated: i) cultivation, ii) juice extraction, iii) fermentation, and iv) distillation. Bioethanol is characterized as being high in energy, 26.6 MJ/kg. For this reason, 1 MJ was selected as the functional unit (FU) (Consorcio 2012).

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2.1.2. System boundaries and assumptions

The LCA carried out for the bioethanol production system analyzed the entire chain of production, from cultivating sugarcane and agave to producing bioethanol from sugarcane molasses and agave juice. The main inputs in fermentation are generated at the extraction stage at which point molasses and agave juice were produced. Figures 1 and 2 represent the system boundaries considered for producing biofuels from sugarcane molasses and agave juice, respectively, considering the main inputs and outputscorresponding to each stage.

130 The following assumptions were made in this approach:

131 ✓ Chemical, fertilizer, pesticide, and energy production were included within the
 132 system boundaries as "market" dataset. A "market " data set collects all activities with the
 133 same reference product in a certain geographical region, including the average amount of
 134 transport related to this product within that area (Ecoinvent 2019).

135 ✓ Transport of sugarcane and agave to the extraction plant were considered.

136 ✓ The plant extraction and the bio-refinery plant were assumed to be in the same
137 place.

138 ✓ Capital goods, staff and buildings were excluded from this evaluation.

139 ✓ The system boundary excluded the usage and end of life for sugar and bioethanol
140 products.

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2.1.3. Life cycle inventory analysis

The primary inventory data for cultivating and extracting sugarcane and agave
cultivation, sugar, and molasses/agave juice fermentation stages are shown in Tables 1 3, respectively.

In this study, data collected for the raw material, utilities, and products at the cultivation stage were provided from a real plant in Mexico (Veracruz). However, air, water and soil emissions at this stage were calculated according to the Intergovernmental Panel on Climate Change (IPCC), Environmental Protection Agency (EPA) and Ecoinvent (EPA 2016, 2017, Klein et al. 2006, Nemecek &Kägi 2007). In addition, the input and output data for the extraction stage were taken from the literature (Consorcio 2012, Gamboa 2006, Livier 2004, Marín 2014, SAGARPA 2018a). The mass and energy
balances for the biorefinery plants were estimated by simulating the entire process with
Aspen Plus[®] V.9 software (Aspentech, Bedford, MA, USA). Finally, the background
processes were considered from the Ecoinvent database (Ecoinvent 2019).

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a. <u>Block I: Agriculture stage</u>

156 i. Sugarcane

157 In this study, a five-year cycle was assumed for producing sugarcane. In the first year, 158 the soil was prepared (by harrowing, ploughing, and raking). Next, 20,000 kg/ha of 159 compost were used for soil conditioning, which was transported 25 km from the "La 160 Gloria" sugar refinery to the plot. Apart from compost, in order to make sugarcane 161 productive, it is essential to use fertilizers and pesticides, as crop productivity depends on 162 primary nutrients such as nitrogen, phosphorus and potassium (Meyer 2013). To obtain 163 the greatest yields from fertilizers, these should preferably be used when the soil is humid, 164 as this helps in the dilution and absorption of nutrients (Meyer 2013). Specifically, in this 165 study, fertilization was performed annually, and fertilizers and pesticides were 166 transported 7 km in a 3-tonne truck. The ones used were: Triple17 (300 kg/ha), urea (150 167 kg/ha), Allectus 300sc (12 kg/ha) and Engeo (12 kg/ha).

Furthermore, the crop was irrigated with a gravity-fed system, using water from a river located 2 km away from the plot. Harvesting was performed manually, and the sugarcane was transported by truck to the mill, which was 25 km away. Total yields per annum were as follows: 1st year 140 tons/ha, 2nd year 120 tons/ha, 3rd year 100 tons/ha, 4th year 90 tons/ha and 5th year 85 tons/year.

173 ii. Agave Salmiana

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174 Agave Salmianais is used for producing alcoholic and non-alcoholic drinks. In this 175 research, a 6-year cycle was assumed for agave cultivation. In the first year, the soil was 176 prepared by harrowing. Planting was carried out in a rectangle (plants placed 3 meters 177 apart), which yielded an average of 1,200 plants/ha.

178 The main advantage of using this plant is that it can be grown on highly degraded 179 soils that are poor in nutrients and water (Davis et al. 2011). Pruning, which consisted in 180 removing the outer leaves, which were already adult and dry, was carried out every two 181 years. Here, fertilization was performed manually every year, with 4 tons/ha of compost 182 made up of glyphosate (3 kg/ha), bifenthrin (20-30 kg/ha), and copper sulphate (3 kg/ha) 183 during the rainy season. In addition, throughout the cultivation period, the crops were 184 rain-fed only. Agave yielded 1,200 plants/ha whose average weight was around 250 185 kg/plant.

186 b. Block II: Raw material processing stage

187 i. Sugar extraction

188 After transporting the sugarcane to the sugar extraction plant, it was weighed and then 189 stored in baskets (Consorcio 2012). The sorted sugarcane was then transported in a 190 conveyor belt system to choppers whose blades were used for splitting it. Next, it was 191 crushed in six mills with three or four maces to extract the juice (Consorcio 2012). 192 Meanwhile, water was added to extract the sucrose contained in the fibrous material, and 193 the juice and bagasse were obtained at this point. The latter was evacuated in the fourth 194 mill (Consorcio 2012). In order to reduce costs and the environmental impact, 50% of the 195 bagasse was used as a fuel for generating electricity (Consorcio 2012). The rest was used 196 as a raw material in thermochemical processes.

197 Subsequently, the resulting juice was weighed to define the proportion of calcium 198 oxide to be added, and this mixture was heated to 102-105 °C. Afterwards, came 199 clarification at which point the juice was purified, with all impurities removed in the form 200 of insoluble calcium salts (Consorcio 2012). Sucrose was then recovered from these solid 201 impurities by filtration, to obtain juice and a solid by-product (sugarcane press-mud) 202 which can be used as compost (Consorcio 2012, Sanchez et al. 2017).

The filtered juice, whose sugar content was about 14 wt.%, was subjected to evaporation in an evaporation train to remove any excess water and to gain 60 wt.% solids (syrup) (Consorcio 2012). This syrup was then crystallized in three tanks in a vacuum. The liquid and solid phases were next separated by centrifugation to yield sugar and molasses (Consorcio 2012).

208

ii. Agave juice extraction

209 On maturity the agave plant was harvested by removing the leaves until the center of 210 the plant (which is called the *pineapple*) was reached (L. Gutiérrez-Coronado et al. 211 2007). Firstly, this was cooked in an autoclave using pressurized saturated steam (Livier 212 2004). The cooking by-product (syrup) was then collected in a tank. Next, the cooked 213 pineapple was ground to obtain cut agave and organic waste. The former was washed to 214 extract the first syrup while the organic waste (wet bagasse) was sent to the second mill. 215 The second and third milling were carried out under the same conditions as the first one 216 in order to obtain syrup and bagasse (Livier 2004). The three syrups obtained were called 217 agave juice, which were then stored in a tank and fermented to obtain bioethanol. At this extraction stage, 50% of the resulting bagasse and 10 kg of coal were used to produce the 218 219 electricity needed (Consorcio 2012).

220 c. <u>Block III: Biorefinery plants</u>

In this paper, bioethanol produced from molasses and agave juice was yielded at various stages. During fermentation (first stage), microorganisms, the most commonly used of which were yeasts (e.g. *S. cerevisiae*) (Robak &Balcerek 2018), converted sugars (glucose and fructose) into bioethanol and CO₂ (Equation 1) (Lin &Tanaka 2006).

225
$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$$
 (1)

Distillation was the second stage and the aim of which was to obtain anhydrous bioethanol concentrated up to approximately 96%. The drawback to this was the large amount of energy used (Gavahian et al. 2016).

The final stage was dehydration in which anhydrous ethanol (i.e. 99.7 wt. %) was obtained by using molecular sieves (Robak &Balcerek 2018, Soreanu et al. 2004).

In this study, bioethanol production was simulated in Aspen Plus and using the Nonrandom two-liquid (NRTL) method. Table 4 shows the features of both the sugarcane molasses and agave juice employed in this study.

Table 5 gives a brief explanation of each block used for simulating bioethanol production. The flowsheet diagrams for obtaining bioethanol from sugarcane molasses and agave juice are shown in Figure 3.

The difference between simulations was water requirements. This must be added to prevent yeast cells dying on account of the high osmotic pressure of the fermentation culture (Jambo et al. 2016). Indeed, sugarcane molasses, whose sugar concentration was 48.7 wt.% (Table 4), needs to be diluted until 30 wt.% is reached, whilst agave juice does not as it is lower in sugars (i.e., 9.8 wt.%).

Fermentation was the first stage and was simulated by means of a RSTOIC at 30 °C.
In the fermenter, sucrose was converted to ethanol to obtain 14 wt.% and 4.7 wt.% ethanol

for molasses and agave juice, respectively. In this study, it was assumed that sucrose was converted into glucose and fructose at a rate of 100%, while the rate for converting glucose and fructose into bioethanol and CO₂ was assumed to be 85.7%. (Ghani &Gheewala 2018).

248 The resulting CO₂ was removed in Sep-CO₂ equipment, while the remaining stream 249 was heated to 85 °C. After heating, distillation was performed with two rectification 250 columns (Rectif1 and Rectif2). In the former, 15 stages were employed, while the latter 251 used 50. Feeding for the first column occurred at the 6th stage, while for the second column, it was the 49th. From the first column, bioethanol was obtained with 50 wt.% and 252 253 45 wt.% for molasses and agave juice, respectively. In the second column, the bioethanol 254 was purified at 94 wt.%, a value close to that for azeotropic bioethanol (95.6 %) (Valencia 255 &Cardona 2014). The by-product obtained in the first distillation unit (vinasse) was 256 considered to be an avoided product.

The distilled stream was heated to 115 °C and introduced into the dehydration zone, which is commonly carried out with molecular sieves. In this study, these were modeled as a separator column. The resulting stream (i.e., 99.9 wt.% ethanol) was cooled (Cooler2) to 50 °C whereas, the output streams (i.e. emissions, water, and ethanol) were cooled (Cooler1) to 70 °C. Moreover, steam and cooling water were employed as the heat source for both distillation columns. In this study steam was obtained by a water heater, while river water was used for cooling.

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2.1.4. Impact assessment methodology

The LCA was carried out using the SimaPro 8 software, with the ReCiPe 2016 Midpoint (H) methodology to calculate the LCA results. The following impact categories were selected for determining the environmental performance of the bioethanol produced:

268	GWP, ozone depletion potential (ODP), photochemical oxidation formation potential -
269	humans (HOFP), photochemical oxidation formation potential - ecosystems (EOFP),
270	terrestrial acidification potential (TAP), freshwater eutrophication potential (FEP),
271	human toxicity potential - cancer (HTPc), human toxicity potential - non-cancer (HTPnc),
272	fossil fuel potential (FFP) and WCP.
273	In the chain of production for bioethanol, different by-products were obtained.
274	Therefore, economic allocations were used for the environmental burdens of co-products
275	(Ecoinvent 2019). The economic allocation factors were:
276	✓ Sugar extraction: 80.6 % (0.58 €/kg) for sugar, 8.6 % (0.19 €/kg) for sugarcane
277	molasses, 8.95 % (0.025 €/kg) for sugarcane press-mud and 1.85 % (0.01
278	€/kg).
279	✓ Juice extraction: 99.3 % (0.2 €/kg) for agave juice and 0.7 % (0.01 €/kg).
280	✓ Bioethanol production (molasses): 82.4 % (0.75 €/kg) and 17.6 % (0.025
281	€/kg).
282	✓ Bioethanol production (molasses): 57.4 % (0.75 €/kg) and 42.6 % (0.025
283	€/kg).
284	2.2. Preliminary costs analysis
285	A preliminary cost analysis was carried out to determine the economic feasibility of
286	producing bioethanol from sugarcane molasses and agave juice. An economic evaluation
287	was made using the percentages methodology (Hillstrom &Hillstrom 2002, Peters et al.

288 2003). The Aspen Plus® software was used for assessing the financial aspects related to
289 equipment costs. In addition, the price of the storage tank was calculated according to its

290 scale (Kalk &Langlykke 1986). The evaluation corresponded to V class evaluation

economy. This approach is commonly used for screening alternatives and all cost
estimations were accurate between 30% and 50% (Becerra et al. 2017, Proaño et al. 2020).

Furthermore, by observing the quantity of utilities needed in the process, water and energy costs could be estimated. The sale price of the products (bioethanol and vinasse) also had to be set. The financial indicators considered in this study were the following: net present value (NPV), internal rate of return (IRR) and payback.

297 3. Results

298 In this research, an environmental and economic analysis was performed to determine 299 the most suitable crop for producing bioethanol. In this study, sugarcane molasses and 300 agave juice were used as feedstock. The stages involved in converting these to bioethanol 301 as well as the scenarios overall were compared. The conversion stages included 302 cultivation, extraction, and biorefining. Moreover, an economic and sensitivity analysis 303 of the bioethanol production stage was made to determine which of the two crops was 304 more economical viable. In the following section, the environmental impacts for both 305 feedstocks are shown.

306 **3.1. Producing bioethanol from sugarcane molasses**

307 In this section, the results for the 'cradle-to-gate' analysis for producing bioethanol 308 from sugarcane molasses are shown in Figure 4. In addition, the LCA results for each 309 analyzed stage presented in Table 6.

According to Figure 4, sugarcane extraction showed the greatest results in almost all impact categories whose values were higher than 45%. It had the highest impact on HTPnc (47%) whereas bioethanol production showed the lowest contribution in all categories (<15%). Concerning GWP, significant differences were observed among stages according to Table 6. Thus, sugar extraction had the highest impact value (1.82 kg CO₂ eq) followed by sugarcane cultivation (1.04 kg CO₂ eq) and bioethanol production (3.99E-01 kg CO₂ eq). The results obtained for the former were mainly due to the high amounts of CO₂ given off (Table 2) and background processes (quicklime and coal production). Also, the GWP impact value obtained for sugarcane cultivation was associated with the GHG given off and the diesel used in transport (Table 1).

320 Like GWP, FEP and FFP showed the same tendency. In this respect, the values 321 obtained at sugar extraction in terms of FEP and FFP were 9.38E-05 kg P eq and 3.19E -322 01 kg of oil eq, respectively. The SimaPro software identified that the main contributing 323 factors to FEP at the second stage were background processes, such as coal production 324 and emissions during these processes. In terms of sugar extraction, using and producing 325 coal for obtaining energy and steam were found to be the factors which had most impact 326 on FFP. Moreover, the negative impacts on both categories were also due to P_2O_5 327 emissions, the use of diesel, P-based fertilizers, and compost (Table 1).

328 The high environmental impact on cultivating sugarcane was due to emissions from 329 organic and inorganic fertilizers, water, and the diesel used. In ODP, the most influential 330 factors were N₂O emissions from N-based fertilizers and compost, and the CH₄ given off 331 from transport from burning diesel (Table 1) (Papong et al. 2017). For HOFP and EOFP, 332 the impacts with sugarcane cultivation (Table 6: 1.80E-03 and 1.85E-03 kg NO_x eq. 333 respectively) were associated with NOx emissions from transport and background 334 processes (energy and diesel production) (Table 1). NH₃ and NO_x emissions from 335 cultivation (transport and using fertilizer and pesticide) were the main contributors to 336 TAP. In addition, SO_x emissions from fertilizers and energy production (background 337 processes) significantly contributed to this. Also, higher values were observed for HTPnc

than for HTPc for sugarcane cultivation (Table 6). According to SimaPro's data, these
impacts were mainly associated with background processes (fertilizer and pesticide
production) and emissions (e.g., benzene, cadmium, nickel, chromium) (Silalertruksa et
al. 2017). Finally, WCP was affected by the high amounts of water used in irrigation and
preparing fertilizers (Table 1).

343

3.2. Producing bioethanol from agave juice

Figure 5 shows the results for the agave-to-bioethanol chain, considering the ten selected categories. Table 7 presents the LCA results for each stage under consideration in this research. All the impact values at each stage were calculated for 1 MJ of bioethanol produced.

According to Figure 5, bioethanol production contributed to the highest impact in all categories. The values obtained for this were: 72% (GWP), 57% (ODP), 81% (HOFP and EOFP), 79% (TAP), 60% (FEP), 61% (HTPc), 54% (HTPnc) 83% (FFP), and 85% (WCP). Additionally, both cultivation and juice extraction showed similar values in all categories, as shown in Figure 5.

As for agave, bioethanol production was the most environmentally damaging stage. This was associated with the low sucrose concentration and consequently low ethanol yield during fermentation, factors which affected performance. Therefore, a higher amount of both raw materials and utilities were required to produce 1 MJ of bioethanol from agave juice in comparison to sugarcane molasses.

The information generated by SimaPro software indicated that producing and using grid energy to produce bioethanol were the main explanatory factors behind this detrimental environmental impact (Table 3). Energy production, considered to be a 361 background process, had a significant influence on almost all the categories analyzed 362 (GWP, ODP, HOFP, EOFP, TAP, HTPc, HTPnc and FFP), mainly due to the large 363 amount of emissions. For instance, NO_x emissions were observed to be primarily 364 responsible for the values obtained in HOFP, EOFP and TAP. Also, CH₄ emissions 365 (background processes) were detrimental to GWP and ODP (Nguyen & Gheewala 2008, 366 Zhang et al. 2010). The high value of GWP (6.72E-01 kg CO_2 eq) was also due to the 367 CO₂ given off when fermenting agave juice (Table 3) (Amores et al. 2013, González-368 García et al. 2012, Wang et al. 2013). Human toxicity categories were affected by 369 emissions such as those from nickel, cadmium, chromium, and formaldehyde that were 370 given off mainly in energy and chemical production. Raw materials such as coal, natural 371 gas, and oil used in background processes were found to be the main components which 372 influenced FFP. Also, the effect producing bioethanol had on FEP was related to agave 373 cultivation and juice extraction, while WCP was affected by the water consumed at the 374 last stage (Table 3).

375 At the cultivation stage, using fertilizers and transport had a high impact on ODP due 376 to CH₄ and N₂O emissions. According to Table 7, the impact values for HOFP and EOFP 377 were 6.42E-05 and 6.65E-05 kg NO_x eq, respectively, and these were attributed to NO_x 378 emissions (Table 1) given off when raw materials, fertilizers and pesticides were being 379 transported. Transportation, using fertilizers and compost made a significant contribution 380 to TAP as they generated high amounts of NO_x and NH₃ (Table 1). In addition, 381 background processes such as producing fertilizers and pesticides were harmful in terms 382 of HTPc and HTPnc (Silalertruksa et al. 2017).

383 **3.3. Producing bioethanol from molasses vs. agave juice**

Figure 6 compares the relative environmental impacts for producing bioethanol from sugarcane molasses and agave juice. Table 8 shows the impact values for 1 MJ of bioethanol produced from sugarcane molasses and agave juice.

387 On comparing both scenarios, bioethanol produced from agave juice was seen to make 388 a relatively minor contribution in all categories. However, in the previous analyses, 389 impacts on producing bioethanol from agave juice were observed to be higher than those 390 for molasses. Hence, agave juice is more environmental-friendly. This significant 391 difference could be due to the different ways these raw materials are cultivated and 392 processed. Therefore, in this way, molasses was seen to generate much higher impact 393 values than agave juice (Tables 6 and 7) and, consequently, molasses were more harmful 394 to the environment overall.

When converting sugarcane-to-bioethanol the amount of GHG emissions was 384% 395 396 higher than those for agave-to-bioethanol. Indeed, GHG for sugarcane was 3.26 kg of 397 CO₂-eq/MJ, while for agave; this figure was only 0.67 kg. GHG emissions, as well as 398 using N-fertilizers, coal and energy, increased the value of GWP (Nguyen & Gheewala 399 2008, Pryor et al. 2017, Wang et al. 2012). In addition to CH₄ and N₂O, the data provided 400 by SimaPro indicated that emissions of Halon-1211, Halon-1301, CFC-10 and CFC-12 401 were the most detrimental to the environment in terms of ODP (González-García et al. 402 2012). Also, the impact value obtained in this category could be linked to cultivation. At 403 this point pesticides (which may contain CH₄ and halocarbon compounds) were used. In Table 8, it was observed that the impact value for ODP in molasses was higher than in 404 405 agave juice. This may be because more pesticides were required, and more gases were 406 given off to cultivate sugarcane than agave (Table 1).

407 According to Table 1 and 2, Global NO_x emissions in sugarcane-to-bioethanol 408 were1.86E-05 kg/MJ of bioethanol, while in agave-to-bioethanol, they were 1.22E-04 409 kg/MJ of bioethanol, respectively. Moreover, NO_x, SO_x, NH₃, CO, and hydrocarbons 410 were given off on producing and using fertilizers and pesticides, transport, burning coal 411 and bagasse, and energy production were the main contributing factors to the following: 412 HOFP, EOFP, TAP, as shown in Table 8 (Brizmohun et al. 2015, Costa et al. 2018, Ghani 413 &Gheewala 2018, Ruiz et al. 2018). The higher amount of NO_x given off and greater 414 consumption of these feedstocks (i.e. coal, pesticides, and fertilizer) in sugarcane meant 415 that bioethanol from this raw material had a greater environmental impact in terms of 416 HOFP, EOFP and TAP than agave (Figure 6 and Table 8) (Brizmohun et al. 2015, 417 Michailos 2018)

418 Figure 6 and Table 8 showed that in terms of human toxicity, values for sugarcane 419 were up to approximately 70% higher than they were for agave (78% for HTPc and 89%) 420 for HTPnc). This may be because sugarcane is relatively more reliant on fertilizers, 421 pesticides, coal, and diesel than agave. It was also on account of the high emissions given 422 off with the former (Tables 1-3) (Ghani & Gheewala 2018, Han et al. 2019, Ruiz et al. 423 2018). Moreover, on producing energy, fertilizers, pesticides, chemicals, diesel, coal and 424 compost (background processes), pollutants such as nickel, cadmium, chromium and 425 formaldehyde (that damaged the environment in terms of HTPc and HTPnc) were given 426 off (Brizmohun et al. 2015).

427 In sugarcane cultivation, considerably more fertilizers, pesticides and compost were 428 used. Additionally, this process created the highest amount of wastewater ash and 429 emissions (P_2O_5) (Table 1) all of which led to a greater impact on FEP than agave did 430 (Figure 6 and Table 8) (Brizmohun et al. 2015, Costa et al. 2018, Ghani & Gheewala 2018,
431 Michailos 2018, Ruiz et al. 2018)

Finally, the raw materials used (coal, natural gas and oil) for producing diesel and chemical products were the main contributing factors to FFP (Table 8) (Brizmohun et al. 2015, Ghani &Gheewala 2018). Moreover, the water used in irrigation (sugarcane), preparing fertilizers and pesticides, extracting sugar and agave and producing bioethanol contributed to WCP (Table 8)(Papong et al. 2017). As observed in the other categories,

437 as well as FFP and WCP, sugarcane had higher impact values than agave (Figure 6).

438 **3.4. Recommendations for improving environmental performance**

439 Several recommendations for making bioethanol from sugarcane molasses and agave
440 juice more environmentally-friendly could be considered. One of the greatest challenges
441 to meet is making the raw material more productive without damaging the ecosystem
442 (Farahani & Asoodar 2017, Osei et al. 2003, Papong et al. 2017, Silalertruksa & Gheewala
443 2009, Steiner et al. 2007).

In this respect, soil quality must be improved by substituting inorganic fertilizers with organic ones, such as manure or compost (Osei et al. 2003, Steiner et al. 2007). Also, this would considerably reduce eutrophication (Silalertruksa &Gheewala 2009). Similarly, reducing organic waste and emissions into the atmosphere also improves the environmental performance at the cultivation stage. A decrease in CH_4 , CO_2 , N_2O , and NO_x emissions in turn reduces impact values in terms of GWP, HOFP, EOFP, TAP, among others (Silalertruksa &Gheewala 2009).

451 For sugar and agave juice extraction, coal-produced energy was primarily responsible452 for the negative environmental impact. In this respect, it is recommended substituting coal

with another fuel or using renewable energy such as biomass or hydraulic energy (the
most widespread in Veracruz, Mexico) (CEMAD 2016, Farahani & Asoodar 2017) as this
reduces GHG emissions and environmental damage in sugar extraction.

456 Finally, to reduce the impact that bioethanol production has on the environment; the 457 amount of grid energy consumed must be reduced. In this respect, as in the processing 458 stage, it is recommended replacing grid energy with that generated from renewable 459 sources (biomass or hydraulic). Using renewable energy at the ethanol production stage 460 could help reduce GHG emissions. In this sense, a sensitivity analysis was carried out in 461 which grid energy was increasingly replaced with renewable energy. The main results of 462 these analyses can be seen in Figures 7 and 8 and in Table 9. The sensitivity scenarios are 463 as follows:

464 ➤ Base scenario: 100% grid energy and 0% renewable energy;

465 ➤ Scenario 1: 75% grid energy and 25% renewable energy;

466 ➤ Scenario 2: 50% grid energy and 50% renewable energy;

467 ➤ Scenario 3: 25% grid energy and 75% renewable energy;

468 ➤ Scenario 4: 0% grid energy and 100% renewable energy;

469 Figure 7 and 8 shows that by changing from the Mexican energy grid to renewables, 470 most of these impacts will be significantly reduced. In this research, we assumed that 471 renewable energy would not have an environmental impact. For instance, GWP would be 472 reduced by almost 50%, if the energy came from renewable sources and sugarcane was 473 employed to produce bioethanol. This reduction was based on the fact that the energy grid 474 in Mexico was mainly oil-based (>60%), while renewables still accounted for under 20% 475 (Sarmiento et al. 2019). A reduction in oil consumption would cause a fall in GHG 476 emissions. However, a higher drop would be observed if agave was employed as the 477 feedstock. The relatively higher drop for agave was associated with the energy
478 consumption required to produce bioethanol. According to Figure 1 and 2, producing 1
479 MJ of ethanol from sugarcane and agave would require 1.25 and 1.90 MJ of energy,
480 respectively.

481 Apart from this strategy, using vinasse as compost may significantly reduce 482 environmental damage. It is also essential to capture and store any CO₂ given off on 483 producing bioethanol by means of carbon capture and storage technology (CEMAD 2016, 484 Farahani & Asoodar 2017, Laude et al. 2011, Silalertruksa & Gheewala 2009).

485

5 **3.5.** Comparison with other studies

486 As earlier mentioned, there is little research on producing bioethanol from agave (Yan 487 et al. 2011); However, several articles concerning the environmental screening of 488 bioethanol produced from sugarcane have been published. For instance, Farahani 489 andAsoodar (2017) reported that sugarcane cultivation mainly contributed to 490 acidification, ozone layer depletion, human toxicity and photochemical oxidation. In 491 addition, sugar extraction mainly contributed to global warming potential. Moreover, 492 Amores et al. (2013) demonstrated that sugarcane cultivation is the main hotspot in the 493 life cycle since it affected almost all categories except eutrophication. Similarly, 494 Silalertruksa and Gheewala (2009) observed that it was the main contributing factor to the 495 environmental impact in terms of global warming, photo oxidation, acidification, human 496 toxicity and eutrophication.

497 As observed in this study, cultivation was not the main hotspot when producing 498 bioethanol from sugarcane. In this paper, sugar extraction contributed to a greater extent 499 of the environmental impact than cultivation and bioethanol production. Indeed, it 500 accounted for at least 46% in all the categories assessed. 501 According to the literature review, global warming potential ranged between 0.016 and 502 400 kg CO₂ produced for 1 MJ of ethanol from sugarcane(Amores et al. 2013, Farahani 503 &Asoodar 2017, Silalertruksa &Gheewala 2009, Valencia &Cardona 2014). Table 8 504 shows that around 3.26 kg CO₂-eq/MJ was given off when sugarcane molasses was the 505 feedstock. In other words, it can be concluded that the observed carbon footprint quite 506 similar for that previously reported in others research. These discrepancies in the research 507 were ascribed to i) assessment models (e.g., CML and ReCiPe); ii) allocation method; iii) 508 and inventory data.

509 Furthermore, when comparing the actual study with that of Ghani andGheewala 510 (2018), some similarities can be observed. They studied four different scenarios for 511 producing bioethanol from molasses, the first of which was based on very similar 512 assumptions to those we made. Thus, they considered using inorganic fertilizers and 513 freshwater irrigation for cultivation, bagasse and biogas (from treated wastewater from 514 the bioethanol plant) to produce electricity. Cane waste was burned, wastewater was 515 discharged into surface water and filter cake was used as fertilizer. As in this study, they 516 used the ReCiPe 2016 midpoint methodology and the SimaPro 8.4 software to evaluate 517 impacts. On comparing the results obtained for the five categories in this research and 518 those by Ghani andGheewala (2018), similar values were observed in three of them 519 (GWP, FEP and FFP). The differences seen in the other two (TAP and HTPc) might have 520 been linked to the different assumptions made, such as burning cane waste and producing 521 biogas (Ghani & Gheewala 2018).

As for the ethanol produced from agave, we reported a carbon footprint of 0.70 kg CO₂-eq/MJ, whose value was lower than that reported for sugarcane juice, as shown in Table 8. Considering the agave plant-to-bioethanol production chain, the main stage that 525 contributed to the high environmental impact was producing bioethanol from agave juice. 526 This was mainly attributed to energy consumption on purifying the bioethanol. This stage 527 is known to be one of the main hotspot within the life cycle (Sanchez et al. 2021). 528 However, Yan et al. (2011) reported that crop cultivation was the highest contributing 529 factor to environmental impact in terms of GHG. Furthermore, they reported overall GHG 530 emissions of 0.0044 kg CO_2 -eq/MJ whose value was lower than that reported in this study 531 (i.e. 0.70 kg CO₂-eq/MJ) and our value was higher due to the energy consumed from the 532 Mexican grid.

533 **3.6. Economic analysis**

The parameters considered for carrying out the preliminary economic analysis were as follows: installation capacity of 1000 kg/h of raw material, operating time for the plant of 8000 h/year, total operating time of 15 years, and 50% of total costs would be invested in year zero. The inflation rate was 3.8%, the tax rate was 30% and the depreciation coefficient was 7% (FinancialredMéxico 2018, IPC 2018).

Table 10 shows the costs of equipment and utilities. Table 11 shows a summary of fixed capital, direct production costs and sales of bioethanol produced from molasses and agave juice.

Equipment costs of the biorefinery were provided by the Aspen Plus® economic package, and the storage tank in this study was to scale. Also, working capital was the raw material stock for ten days of production. The bioethanol production plant was assumed to be located in the same place as the agave sugar/juice extraction plant (Veracruz, Mexico), whereby the cost of the raw material was assumed to be zero. In addition, Table 11 shows prices for electricity, water, urea, ammonia sulphate and magnesium sulphate (Budimir et al. 2011, CFE 2019, CONAGUA 2019, SENER 2018). Moreover, it was assumed that six workers, on an annual salary of 15,000 €/worker, were
needed to operate the plant.

Furthermore, Table 11 shows that capital investment, fixed capital and working capital for producing bioethanol from molasses were $1,075,281 \in 860,225 \in and 215,056 \in$, respectively, while for agave juice these figures were $1,036,068 \in 828,854 \in and 207,214 \in$, respectively.

555 On analyzing the data provided by the Aspen Plus simulations, it was observed that 556 from 1,000 kg/h of molasses, 170 kg/h of bioethanol and 1,080 kg/h of vinasse were 557 produced. In comparison, from 1,000 kg/h of agave juice 45 kg/h of bioethanol and 990 558 kg/h of vinasse were produced. The vinasse obtained could not be directly applied to the 559 field, although it could be used in conjunction with other residues from the sugar refinery, 560 and in this way, it could be sold (Consorcio 2012). Both products were put on the market, 561 with the following assumptions on price: 0.75 €/kg for bioethanol and 0.025 €/kg for 562 vinasse (biocompost price) (Castañeda-Ayarza &Cortez 2017, Consorcio 2012).

The results obtained from this economic evaluation indicated that neither of the twobioethanol production scenarios were profitable given that the VPN values obtained were negative (-1,521,947 \in for molasses and -1,785,235 \in for agave juice) and the time for seeing a return on investment was over 15 years. This might have been mainly due to the high amount of energy used to produce bioethanol which entailed high utility costs. In this study, all energy was assumed to be sourced from the grid, with 1600 kW used for sugarcane and 600 kW for agave.

570 Therefore, a sensitivity analysis was carried out in order to evaluate how reliable the 571 project would be if part of the grid energy were replaced by renewable energy, assuming 572 that the latter would cost zero because it would be generated at the plant itself. Energy 573 percentages considered in the sensitivity analysis were the following (Table 12): 574 \blacktriangleright Base scenario: 100% grid energy and 0% renewable energy; 575 Scenario 1: 75% grid energy and 25% renewable energy; Scenario 2: 50% grid energy and 50% renewable energy; 576 \geq Scenario 3: 25% grid energy and 75% renewable energy; 577 \geq 578 Scenario 4: 0% grid energy and 100% renewable energy; \geq

579 \blacktriangleright Scenario 5: NPV=0.

580 The sensitivity analysis showed that varying the energy source had a significant 581 influence on all three economic parameters (Table 12). On analyzing the results, it was 582 observed that if part of the grid energy were replaced with renewable energy, the two 583 bioethanol production processes would become more economically viable. However, 584 there were considerable differences between both scenarios as molasses were more 585 profitable. So, producing bioethanol was only profitable with the ratios 17.1% grid energy 586 and 82.9% renewable energy, and 73.5% grid energy and 26.5% renewable energy for 587 agave juice and molasses, respectively. These considerable differences between both 588 scenarios could be attributed to the lower yields for agave juice in comparison to that for 589 molasses. Hence, producing bioethanol from sugarcane molasses and agave juice was 590 economically viable, better results were achieved with the former.

591 Conclusions

592 This research aims to compare the environmental and economic performance of using 593 sugarcane juice and agave juice as feedstocks to produce bioethanol in Mexico. On the 594 one hand, producing bioethanol from agave juice had a less environmental impact than 595 sugarcane juice. This was ascribed to the low consumption of pesticides, coal, and water 596 throughout the whole chain. Among stages, bioethanol production contributed to a higher 597 extent (>60%) than cultivation and juice extraction due to the low amounts of ethanol 598 yielded in fermentation. On the other hand, the economic analysis revealed that neither 599 of the feedstocks is feasible if the current Mexican energy grid is employed. However, if 600 26.5% of renewable energy is employed along the grid, then producing bioethanol from 601 agave juice would be economical feasible. Briefly, using agave juice, rather than 602 sugarcane molasses as a feedstock for producing bioethanol seems to be more promising 603 from an environmental and economic point of view. On a final note, in Mexico it would

- be worthwhile creating robust policies to encourage the adoption of renewable energy.
- 605 Acknowledgments

606 The authors would like to thank the University of Castilla-La Mancha ,Spain for their

607 financial support (UCLM "Plan Propio de I+D+i. (2016 / 14100)" Grant). The authors

acknowledge the financial support given by the Castilla-La Mancha regional government

609 (Project SBPLY/17/180501/000238).

610 **Data availability**

All data generated and analysed during this study have been included in this publishedarticle.

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813	Ethical Approval
814	Not applicable
815	Consent to Participate
816	Not applicable
817	Consent to Publish
818	Not applicable
819	Authors Contributions
820	Maria Magdalena Parascanu: investigation, writing and preparing original draft, data
821	curation, editing. Nestor Sanchez: data curation, simulation, editing. Fabiola Sandoval-
822	Salas: data curation, research. Carlos Mendez Carreto: formal analysis, research.
823	Gabriela Soreanu: conceptualization, reviewing, supervision.Luz Sanchez-
824	Silva:conceptualization, funding acquisition, visualization, project administration.
825	Conflict of interest

826 The authors declare there to be no conflict of interest.