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# Simultaneous Life Cycle Assessment and Process Simulation for Sustainable Process Design

**Simone C. Miyoshi and Argimiro R. Secchi ***

Chemical Engineering Program, COPPE, Universidade Federal do Rio de Janeiro, Cidade Universitária,
Rio de Janeiro 21941-972, Brazil; smiyoshi@peq.coppe.ufrj.br
* Correspondence: arge@peq.coppe.ufrj.br

**Abstract:** While there are software tools available for helping to conduct life cycle assessment (LCA), such as OpenLCA, these tools lack integration with process design, simulation, and optimization software. As LCA has a critical role in sustainable product design, this paper presents a platform called EMSO_OLCA, which integrates the LCA provided by OpenLCA into the Environment for Modeling, Simulation, and Optimization (EMSO). EMSO_OLCA incorporates a database of environmental impact assessment methodologies from OpenLCA and aligns with the principles of LCA outlined in ISO 14040 and ISO 14044. Validation tests were conducted to compare the results obtained by the LCA of sugarcane ethanol using OpenLCA and EMSO_OLCA, revealing a high level of agreement. The average relative error was 0.045%, indicating a negligible discrepancy between the tools. Moreover, it took only 0.3 s for the calculation, which is desirable for use with process system engineering tools. A second case study was applied to combined steam and electricity production from the combustion of sugarcane bagasse and straw in a combined heat and power system. The results show the integration of LCA with simulation and sensitivity analysis tools, thus supporting sustainable decision-making processes. EMSO_OLCA bridges the gap between LCA and process engineering, enabling a holistic approach to the sustainability, design, and implementation of environmentally friendly solutions.

**Keywords:** process simulation; sensitivity analysis; OpenLCA; EMSO; EMSO_OLCA

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## 1. Introduction

Life cycle assessment (LCA) is a powerful tool used to assess the environmental impact of processes and products. It involves analyzing the material and energy flows throughout the entire life cycle of a product, such as from cradle to grave or cradle to gate, enabling the quantification of the impacts and identification of bottlenecks and improvement opportunities of the environmental performance. It quantifies the environmental impact of a set of elementary processes throughout the life cycle of a product. ISO 14040 [1] provides general guidelines for conducting LCA, and defines LCA as the "compilation and evaluation of the inputs, outputs, and potential environmental impacts of a product system throughout its life cycle". The life cycle includes the utilization of natural resources for the production of inputs and products, transportation stages, product use, and final disposal.

In the transition to a low-carbon economy, the LCA of a productive process becomes of fundamental importance. LCA enables the identification of bottlenecks and improvement opportunities in terms of environmental aspects throughout the life cycle of a production process. It can assist the design of an industrial process by comparing the environmental impact caused by different technological routes. This tool can help in a decision-making process or can even be used for marketing purposes, showing that a process is really green.

Despite the availability of various LCA tools like OpenLCA® [2], SimaPro® [3], and LCA For Experts® [4], these software platforms lack integration with modeling, simulation, and process optimization environments. Previous studies integrating LCA with process simulation have not employed a structured approach that allows the direct integration of LCA software with a process simulator [5–7].

Kalakul et al. [8] developed an LCA calculator (LCSoft) integrated with a process simulation tool. However, it did not represent an integration of LCA software that includes a comprehensive database and LCA methodologies. Thus, there were some discrepancies between the results from SimaPro and LCSoft. Furthermore, the calculated values were not widely integrated within the simulation environment.

The structured integration of life cycle assessment calculations into modeling, simulation, and process optimization environments creates a powerful tool for the development of cleaner processes. A structured integration allows consistency of the LCA through a proper query of the inventory databases with assessment methodologies. This consistency is fundamental to guarantee that the LCA is properly evaluated according to each methodology of impact factors. This type of tool not only provides a way for monitoring emissions throughout the product life cycle, but also offers valuable metrics for determining the most sustainable process design.

The Life Cycle Inventory (LCI) involves data collection and calculations to quantify the inputs and outputs of the defined product system. The ISO 14040 also states that all mass and energy flows should be considered, including different raw materials and energy sources used, as well as the efficiency of energy conversion.

In Life Cycle Impact Assessment (LCIA), various methodologies have been developed. Among the existing methodologies, two main approaches are used to classify and characterize environmental impacts: the problem-oriented approach (midpoint) and the damage-oriented approach (endpoint). Among the methodologies are the CML-IA [9] and ReCiPe [6] approaches. Table 1 presents some impact categories and their respective baseline characterization factors from CML-IA baseline, impacts and effects, main impact substances, and unit of measurement.

**Table 1.** Some impact categories of CML-IA baseline method [9].

| Impact Category (Baseline Charact. Factor) | Impacts and Effects | Main Impact Substances | Unit |
|---|---|---|---|
| Global warming (GWP 100a) | Impact of human emissions on the radiative forcing on atmosphere. Adverse impacts on ecosystem and human health. | $CO_2$, $N_2O$, $CH_4$ | kg $CO_2$-eq |
| Ozone layer depletion ($ODP_\infty$) | Reduction of the stratospheric ozone layer, increasing the UV-B radiation to earth surface. Potential harms to human, animal health and terrestrial and aquatic ecosystems. | Trichlorofluoromethane (CFC-11), Halon 1301, Halon 1211 | kg CFC-11-eq |
| Eutrophication (EP) | Emissions of excessively high level of macronutrients as nitrogen(N), phosphorous (P) and carbon (C) to the environment. Algal Blooms, oxygen depletion. | $NH_3$, P, $PO_4$, $NO_3$, organic matter | kg $PO_4$-eq |
| Acidification (AP) | Damages to the soil, groundwater, surface waters, ecosystems and materials as buildings. | $SO_x$, $NH_x$, $NO_x$ | kg $SO_2$-eq |
| Photochemical oxidation (PCOP) | Emission of photo-oxidant substances. Damage to human health, ecosystems and to agricultural crops. | VOC, CO, $NO_x$ | kg $C_2H_4$-eq |
| Human Toxicity ($HTP_{\infty,global}$) | Impacts acute and chronic toxicity to human health. | Benzene, Cupper, Lead | kg 1,4-DB-eq (1,4-dichlorobenzene) |
| Ecotoxicity | Impact of toxic substances on aquatic, terrestrial and sediment ecosystems. | 1,4-dichlorobenzene, Mercury, Arsenic | kg 1,4-DB-eq (1,4-dichlorobenzene) |

Several software tools, such as OpenLCA® [2], SimaPro® [3], and LCA For Experts® [4], have incorporated Life Cycle Inventory (LCI) databases and impact assessment methodologies.

OpenLCA® is free software for LCA; however, the acquisition of specific database licenses is required. The impact assessment methodologies available in OpenLCA® include CML-IA 2001 [9], ReCiPe 2016 [10], and 99 other methodologies, totaling 1479 impact categories.

This study aims to bridge this gap by proposing the integration of the OpenLCA software's database with the process modeling, simulation, and optimization tool EMSO® [11]. A dedicated tool for integrating these two software platforms has been developed.

EMSO® is an open environment for process modeling, simulation, and optimization with an equation-oriented approach and object-oriented modeling language [11]. EMSO® [11] offers seamless integration with OPC® [12], Python® 3.0 [13], Matlab® [14], Scilab® [15], Excel® [16], and LibreOffice® [17], and provides easy integration with real-time industrial systems.

The proposed tool, EMSO_OLCA, enables several valuable functionalities, including real-time emission monitoring, optimal process design considering environmental parameters, the techno-economic environmental analysis of processes, and the optimization and control of processes guided by environmental metrics. The main advantage is that the tool is totally integrated to the EMSO's environment, allowing the LCA results to be solved simultaneously to the process simulations, design, optimization, sensitivity analysis, and parameter estimation.

## 2. Methodology

### 2.1. EMSO_OLCA

The EMSO_OLCA tool was developed in C++ and follows the structure defined by ISO 14040 [1] Life Cycle Assessment—Principles and Framework, and ISO 14044 [18] Environmental management—Life cycle assessment—Requirements and guidelines. This tool integrates EMSO with the LCA methodologies available in the OpenLCA 1.10.1, and the calculation of inputs is obtained from the LCIA database of process inputs. It leverages the comprehensive database provided by OpenLCA. Additionally, since the impact assessment databases are provided by OpenLCA, they are automatically updated by OpenLCA, thus eliminating the need for separate database updates.

The requirements for using the EMSO_OLCA tool are as follows:

- Obtain the LCIA methods from the OpenLCA Nexus website. These files are proprietary to OpenLCA, but are available free of charge.
- Select and export the impacts of process inputs in OpenLCA 1.10.1 to a .csv file using the provided export functionality.

The information flow in the EMSO_OLCA tool is bidirectional between EMSO and EMSO_OLCA. The user sets the EMSO_OLCA User Configuration that informs the LCA inventory, the methodology, and the characterization factors in EMSO, which are passed down to EMSO_OLCA. EMSO_OLCA then queries the LCIA database and retrieves the impact factors based on the characterization factors defined by the user. EMSO_OLCA also searches for the file containing the pre-calculated impact assessment of inputs, which is generated by a Python application in OpenLCA, as illustrated in Figure 1.

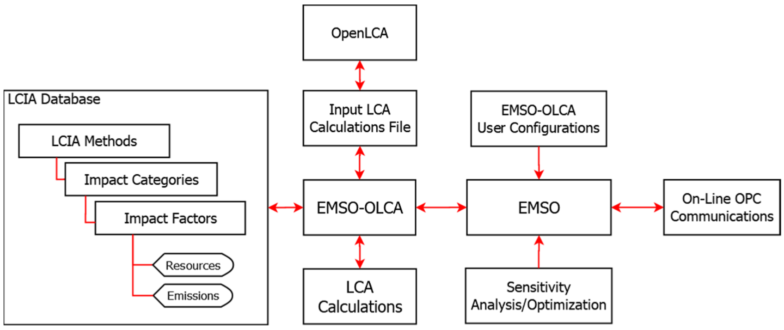


**Figure 1.** Information flux in EMSO_OLCA.

As in Figure 1, EMSO-OLCA performs the LCA calculations, which are directly available within the EMSO environment. This integration enables the extensive utilization of the sensitivity analysis and internal optimization tools provided by the simulator. Moreover, EMSO allows communication-obtained LCA values through industrial protocols such as OPC and Python.

In the user settings, it is necessary to fulfill the information related to the LCA scope and inventory: the functional unit is defined, as well as the impact methods, impact categories, and the LCIA database path. The user settings also include the type of methodology (attributional or consequential), the type of allocation, and the path of the file containing the pre-calculated inputs. The user configuration syntax is presented in Box 1.

**Box 1.** User configuration syntax for EMSO_OLCA (# starts a line comment).

```
obj as Plugin (Type= "EMSO_OLCA",
DataBasePath=[‘‘C:/Users/usuario/Documents/EMSO_OLCA/methods_database’’],
MethodName= ["MethodName"],
ImpactCategory=["ImpactCategory1", "ImpactCategory2"],
InputFileName=[‘‘C:/Users/usuario/Documents/EMSO_OLCA/export_input.csv’’],
Inputs=["name of input1", "name of input 2"],
OutputName=["name of the output 1"],
OutputUnit=["kg"],
ElementaryFlows=["Emission1","Emission2",‘‘ResourceName1","ResourceName2"],
ElementaryFlowPath1=["Emission to air", ‘‘Emission to air’’, ‘‘Resource’’,
‘‘Resource’’],
ElementaryFlowPath2=["low population density","low population density","in water",
"land"],
UnitFileName=["C:/Users/usuario/Documents/EMSO_OLCA/EMSO_OLCA_units.csv"],
MethodologyType=["attributional"], # ou ‘‘consequential’’
AllocationType=["mass"]); # ou ‘‘energy’’ ou ‘‘economic’’
```

The inventory of a product system is defined by the user, which englobes inputs of energy, inputs of raw materials, outputs as products and co-products, and elementary flows. The elementary flows include emissions to the atmosphere, water and soil, waste, and use of natural resources, as depicted in Figure 2. All of the names of the inputs, outputs, and elementary flows are defined in the user settings as well as the inventory quantities, which can be associated with the simulation variables, ensuring mass and energy balances.

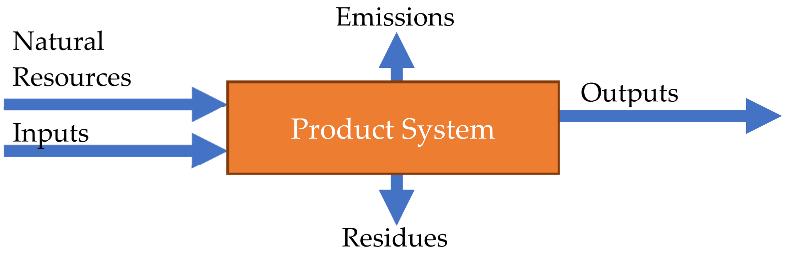


**Figure 2.** General schematic diagram of elementary process.

For calculation purposes, each impact assessment methodology has associated impact categories. Category "*c*" defines a specific impact factor for each component "*i*" ($IF_{c,i}$). The total impact value of category "*c*" ($LCIA_c$) is obtained by multiplying the impact factor $IF_{c,i}$ of component "*i*" for category "*c*" with the quantity of component "*i*" emitted ($LCI_i$), as shown in Equation (1) [19].

$$LCIA_c = \sum_i IF_{c,i} \cdot LCI_i \tag{1}$$

The impact factor values for the inputs are obtained through the OpenLCA software and exported as a .csv file. The OpenLCA links the elementary flows emitted during the life cycle of the input production and exports the results to the .csv file. For emissions and residues emitted during the process, the impact factor is directly obtained from the impact factor database for each impact.

There is an allocation option for multi-product systems using the attributional approach. In this case, the total impact value of category "*c*" is multiplied by the allocation factor $\left(f_p\right)$. The calculation of the allocation factor is given by Equation (2) [9]:

$$f_p = \frac{par_p \cdot q_p}{\Sigma_j \left(par_j \cdot q_j\right)} \tag{2}$$

where the product quantity is given by $q_p$, and $par_p$ is the allocation parameter for each product of the product system analyzed. The denominator is the sum of the product of the quantity multiplied for the allocation parameter. For mass allocation, $q_p$ is mass and the allocation parameter ($par_p$) is set to 1 for all products. This means that the impact of the category is evenly distributed among the different products based on their mass. For energy allocation, $q_p$ can be mass and the allocation parameter ($par_p$) can be set to the energy content of each product (in MJ/kg), for example. This means that the impact of the category is allocated to the products based on their energy content. For economic allocation, the allocation parameter ($par_p$) can be set to the price of each product (in USD/kg). This means that the impact of the category is allocated to the products based on their economic value or price.

## *2.2. Validation and Process System Application Examples*

Biofuels and by-products have also gained interest as they play significant roles in sustainable development and the circular bioeconomy. Section 2.2.1 discusses a validation test conducted to examine the calculation error of the EMSO_OLCA tool in comparison to the values obtained from OpenLCA applied to the inventory of ethanol production in autonomous units.

While novel technologies for sugarcane waste and by-products are still in the research and development stage with promising futures, other well-established methods are already in use for the valuation of waste and by-products from the processing of sugarcane [20,21]. Typically, sugarcane bagasse is used as fuel in cogeneration facilities to produce combined heat and power. Section 2.2.2 shows an LCA case study applied to this type of system.

### 2.2.1. Validation of EMSO_OLCA Compared to OpenLCA

In the implementation of the validation test of the EMSO_OLCA tool, the EcoInvent 3.8 [22] database inventory was used for a case study of ethanol production for autonomous units as a reference. The results obtained from OpenLCA and EMSO_OLCA were compared. In this test, the CML-IA 2016 baseline methodology [23] was used with all of the characterization factors associated with this method.

### 2.2.2. Combined Heat and Power (CHP) Study Case

A case study was also conducted on the LCA of a bioenergy and steam cogeneration unit. Scenarios for bioenergy and steam production from sugarcane bagasse and straw were compared. The composition of sugarcane bagasse was 42.19% cellulose, 27.60% hemicellulose, 21.56% lignin, 5.63% impurities, and 2.84% ash [24]. The composition of the straw was 46.05% cellulose, 27.20% hemicellulose, 24.67% lignin, and 2.08% ash [25]. Oliveira et al. [26] estimated the availability of sugarcane bagasse at 153 kg per ton of sugarcane with a 10% moisture content and 94 kg of straw per ton of sugarcane with a 10% moisture content.

The parameters adopted in the boiler simulation were as follows: boiler efficiency based on the lower heating value of 87.2%; gas outlet temperature of 160 °C; produced steam pressure and temperature of 65 bar and 485 °C; and excess air of 30% [27,28]. The high heating value (HHV) of cellulose, hemicellulose, and lignin were 17,299 kJ/kg, 17,719 kJ/kg, and 26,924 kJ/kg, respectively [27]. A turbine efficiency of 85% and generator efficiency of 98% were assumed [28]. The steam demand for a first-generation ethanol plant (1G) is 370.5 kg of 2.5-bar steam per ton of processed sugarcane [29]. The plant operates 80% of the time during 210 days in a year for a horizon of 25 years [29].

Two scenarios were considered for this steam demand. In the first scenario, the quantity of bagasse and straw was designed to meet the steam demand, using a 65-bar boiler. In the boiler, biomass is burned with excess air to produce superheated steam at 65 bar. The steam is directed to a three-stage turbine, producing electricity. After reaching a pressure of 2.5 bar, liquid water is added to obtain saturated steam. The steam is then directed to the process, releasing its latent heat and returning as saturated liquid. This liquid is added to the water makeup, which is directed to a deaerator receiving a small amount of steam at 2.45 bar, resulting in saturated liquid, which is compressed and returned to the boiler. A simplified diagram is presented in Figure 3.

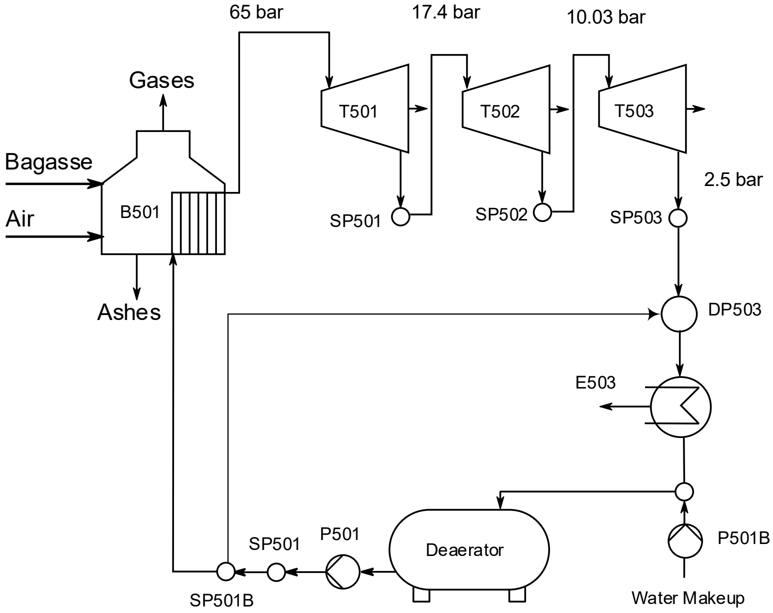


**Figure 3.** Simplified diagram of combined heat and power unit (Scenario 1).

In the second scenario, an additional condensing turbine was added to the three-stage turbines, utilizing all available sugarcane bagasse and straw for power generation. As there is also steam generation in the condensing cycle, the heat produced in the condensing turbine is directed to a cooling tower. The diagram for this scenario is presented in Figure 4.

In the case of cogeneration without a condensing turbine, Scenario 1, the objective of the combined heat and power unit is to meet the ethanol heat demand requirement. On the other hand, in the case of cogeneration with a condensing turbine, the objective of the plant is to increase the production of surplus electricity by burning the bagasse and straw available. Considering the cogeneration process without a condensing turbine, the generated steam is sent to three back-pressure turbines, where the steam produced in one of the turbines is directed to the process units. In Scenario 2, there is no utilization of the steam from the condensing turbines; thus, the heat is compensated by a cooling tower unit.

The simulation of the case studies was implemented in EMSO, and the environmental impact was assessed simultaneously in EMSO and OpenLCA using the EMSO_OLCA tool. For the LCA analysis, the methodology used was also the CML-IA 2016 baseline [23], incorporating all corresponding characterization factors in the attributional approach. The inputs considered were sugarcane bagasse and water. The outputs considered were the heat of the 2.5 bar steam in MJ and net electricity production, taking into account the energy consumption of pumps and the water-cooling tower (if applicable).

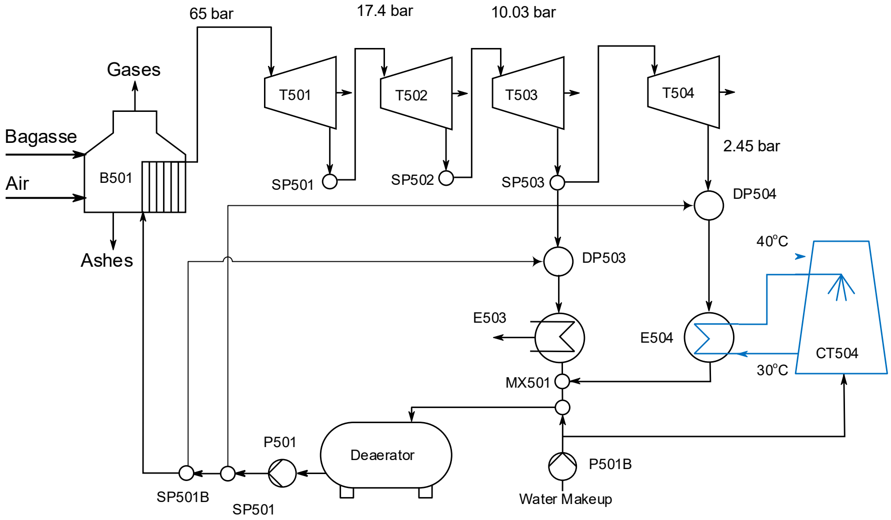


**Figure 4.** Simplified diagram of combined heat and power unit with condensing turbine (Scenario 2).

The emissions resulting from the combustion of bagasse and straw were referenced based on Greet 2020 [30], and the combustion of biogenic $CO_2$ was obtained from the simulation. The reference for each emission considered is also presented in Table 2.

**Table 2.** Emissions related to biomass burning in boilers.

| Emission | Elementary Flow [2] | Type of Elementary Flow [2] | Value [1] | Unit |
|---|---|---|---|---|
| VOC | NMVOC, non-methane volatile organic compounds, unspecified origin | Emission to air | 0.61499 | g/MMBtu |
| CO | Carbon monoxide | Emission to air | 9.7514 | g/MMBtu |
| $NO_x$ | Nitrogen oxides | Emission to air | 64.213 | g/MMBtu |
| PM2.5 | Particulates, <2.5 µm | Emission to air | 1.2671 | g/MMBtu |
| PM10 | Particulates, <10 µm | Emission to air | 1.4347 | g/MMBtu |
| $SO_x$ | Sulfur oxides | Emission to air | 58.923 | g/MMBtu |
| BC | Black Carbon | Emission to air | 0.17486 | g/MMBtu |
| OC | Organic Carbon | Emission to air | 0.41308 | g/MMBtu |
| $CH_4$ | Methane | Emission to air | 9.8650 | g/MMBtu |
| $N_2O$ | Dinitrogen monoxide | Emission to air | 6.1070 | g/MMBtu |
| $CO_2$ | Carbon dioxide, biogenic | Emission to air | from simulation | - |

[1] From Greet 2020 [30]. [2] As in OpenLCA LCIA database.

From the simulation and estimation of emissions, the life cycle inventory of each simulated scenario was obtained. The scope of the LCA was cradle-to-gate. The categories and methodology applied were all categories of CML-IA baseline [23] methodology. The EcoInvent 3.8 database [22] was employed to assess the impacts of the inputs. The allocation was energy-based. It also identified the percentage each input and emission contributed to the obtained LCA result.

A simplified economic analysis was also performed to estimate the net revenue of the steam production system. For the prices of bagasse, water, and energy, the average value in US dollars over the past 5 years was used for the Brazilian market, as shown in Table 3.

**Table 3.** Products and raw material average prices.

| Product/Raw Material | Price | Unit | Source |
|---|---|---|---|
| Water ($p_{water}$) | 0.005235 | USD/kg | [31,32] |
| Electricity ($p_{elec}$) | 59.50 | USD/MWh | [33] |
| Low Sugarcane Bagasse Price ($p_{bag.}$) | 14.58 | USD/t | [5] |
| High Sugarcane Bagasse Price ($p_{bag.}$) | 158.75 | USD/t | [34] |

This analysis considered the process revenues and raw material costs per GJ of steam produced, as shown in Equation (3).

$$NetRev\ (\$/\mathrm{GJ}) = \frac{Surp.\ Elect.\ (\mathrm{kWh}) \times p_{elec}\left(\frac{\$}{\mathrm{kWh}}\right) - Water\ Demand\ (\mathrm{kg}) \times p_{water}\left(\frac{\$}{\mathrm{kg}}\right) - Bag.\ Demand(\mathrm{t}) \times p_{bag.}\left(\frac{\$}{\mathrm{t}}\right)}{Steam\ (\mathrm{GJ}) + Electricity\ Surplus\ (\mathrm{GJ})} \quad (3)$$

A sensitivity analysis was conducted by comparing the results obtained from the life cycle assessment (GWP 100a) and the net revenue varying the steam consumption. This sensitivity analysis was combined in two bagasse prices range: USD 14.58 per ton for low bagasse prices and USD 158.75 per ton for high bagasse prices.

## 3. Results and Discussion

### *3.1. Validation of EMSO_OLCA Compared to OpenLCA*

The results obtained from the comparison between the LCA from the inventory of sugarcane production in autonomous units in Brazil in OpenLCA and the results obtained from the same inventory in EMSO_OLCA applying CML-IA 2016 baseline methodology are presented in Table 4.

**Table 4.** Results from the validation test for LCA of ethanol (autonomous units, BR, 1 kg).

| **Impact Category** | **Unit** | **OpenLCA Results** | **EMSO_OLCA Results** | **Relative Error (%)** |
|---|---|---|---|---|
| Photochemical oxidation | kg $C_2H_4$-eq | 0.00169 | 0.00169359 | 0.2124% |
| Human toxicity | kg 1,4-DB-eq | 0.25019 | 0.250187 | 0.0012% |
| Abiotic depletion | kg Sb-eq | $4.29159 \cdot 10^{-6}$ | $4.29155 \cdot 10^{-6}$ | 0.0009% |
| Eutrophication | kg $PO_4$-eq | 0.00741 | 0.00740821 | 0.0242% |
| Abiotic depletion (fossil fuels) | MJ | 3.28619 | 3.28619 | 0.0000% |
| Marine aquatic ecotoxicity | kg 1,4-DB-eq | 257.255 | 257.255 | 0.0000% |
| Ozone layer depletion (ODP) | kg CFC-11-eq | $1.9625 \cdot 10^{-8}$ | $1.9625 \cdot 10^{-8}$ | 0.0000% |
| Terrestrial ecotoxicity | kg 1,4-DB-eq | 0.00109 | 0.0010923 | 0.2110% |
| Acidification | kg $SO_2$-eq | 0.01395 | 0.0139457 | 0.0308% |
| Fresh water aquatic ecotoxicity | kg 1,4-DB-eq | 0.13882 | 0.138824 | 0.0029% |
| Global Warming (GWP 100a) | kg $CO_2$-eq | 0.06515 | 0.0651403 | 0.0149% |

Table 4 shows that EMSO_OLCA is capable of reproducing calculations from OpenLCA with high accuracy for all categories assessed. The average relative error is 0.045% for the evaluated categories. It is important to note that the computational time required for the calculations was 0.3 s, with a 12th Gen Intel® Core™ i7-12700 processor and 32 GB RAM memory. This time is significantly lower than the OpenLCA, which was about 7.3 s, as a substantial portion of computational time is spent on the preliminary calculation of input impact evaluation. This high computational speed of 0.3 s is a valuable characteristic for real-time applications in process simulators such as EMSO.

### *3.2. Combined Heat and Power (CHP) Study Case*

In order to process a flow rate of 500 t/h of sugarcane, a total availability of 123.5 t/h of sugarcane bagasse and straw is observed. In general, 5% of the available sugarcane bagasse is reserved for unforeseen operational issues and for the start-up of the next harvest season. Thus, the total availability of bagasse and straw is 117.325 t/h. The steam consumption of a 1 G ethanol plant is 370.5 kg of steam at 2.5 bar per ton of processed sugarcane [19]; thus, 185 tons of steam per hour are required, resulting in a demand of 113.35 MW of 2.5 bar steam.

As mentioned in the methodology, two scenarios of combined heat and power were studied: the first scenario considered the production of steam in a 65-bar boiler and electricity in a three-stage turbine and 113.35 MW of 2.5 bar steam. The second scenario included the 65-bar boiler steam production in a three-stage turbine to produce 113.35 MW of 2.5 bar steam, plus a condensing turbine in order to produce as much electricity as possible. The heat produced in the condensing turbine was compensated by a cooling water tower.

The life cycle inventories obtained by supplying 113.35 MW of 2.5-bar steam for both studied scenarios are presented in Table 5.

**Table 5.** Inventory of the LCA of the CHP biomass unit.

| Description | Unit | Scenario 1 | Scenario 2 | Δ% |
|---|---|---|---|---|
| Inputs | | | | |
| Bagasse/Straw | t/h | 37.40 | 117.33 | 214% |
| Water | t/h | 7.46 | 429.11 | 5656% |
| Emissions | | | | |
| VOC | kg/h | 0.36 | 1.13 | 214% |
| CO | kg/h | 5.69 | 17.84 | 214% |
| NO | kg/h | 37.45 | 117.50 | 214% |
| Particulate M., <2.5 µm | kg/h | 0.74 | 2.32 | 214% |
| Particulate M., <10 µm | kg/h | 0.84 | 2.63 | 214% |
| SOx | kg/h | 34.37 | 107.82 | 214% |
| BC | kg/h | 0.10 | 0.32 | 214% |
| OC | kg/h | 0.24 | 0.76 | 214% |
| $CH_4$ | kg/h | 5.75 | 18.05 | 214% |
| $NO_2$ | kg/h | 3.56 | 11.17 | 214% |
| $CO_2$, biogenic | t/h | 60.53 | 189.88 | 214% |
| Products | | | | |
| Vapor | MW | 113.50 | 113.50 | 0% |
| Surplus Electricity, Liq. | MWh | 34.02 | 141.52 | 316% |

As shown in Table 5, the second scenario allows for the combustion of all available straw and bagasse. Therefore, there is a 214% increase in emissions resulting from biomass combustion in the boiler. However, it produces more net electricity, totaling 141.52 MWh of surplus of electricity production. This can be explained because the condensing turbine enables the production of a greater amount of electricity by burning all of the available fuel. Moreover, as the steam generated (in the condensing turbine) is not utilized in the process, it results in an additional quantity of water usage and electricity consumption in the cooling tower. Therefore, this second alternative exhibits higher water, electricity, and fuel consumption; thus, it is not as efficient as the scenario without the condensing turbine.

The life cycle assessment results for each studied scenario, using the CML-IA 2016 baseline [23] methodology, are presented in Table 6.

According to Table 6, there is an increase in all impact categories per MJ of steam and net electricity when the condensing turbine is used. This indicates that the intensity of the use of natural resources is increased with the condensing turbines. This occurs because there is a significant increase in bagasse burning and the heat of this extra stream production is totally wasted. Therefore, by incorporating the condensing turbine, the energy efficiency of 89.5% in Scenario 1 is reduced to 49.6% in Scenario 2. Thus, the use of cogeneration systems with condensing turbines leads to higher natural resource use intensity with lower efficiency.

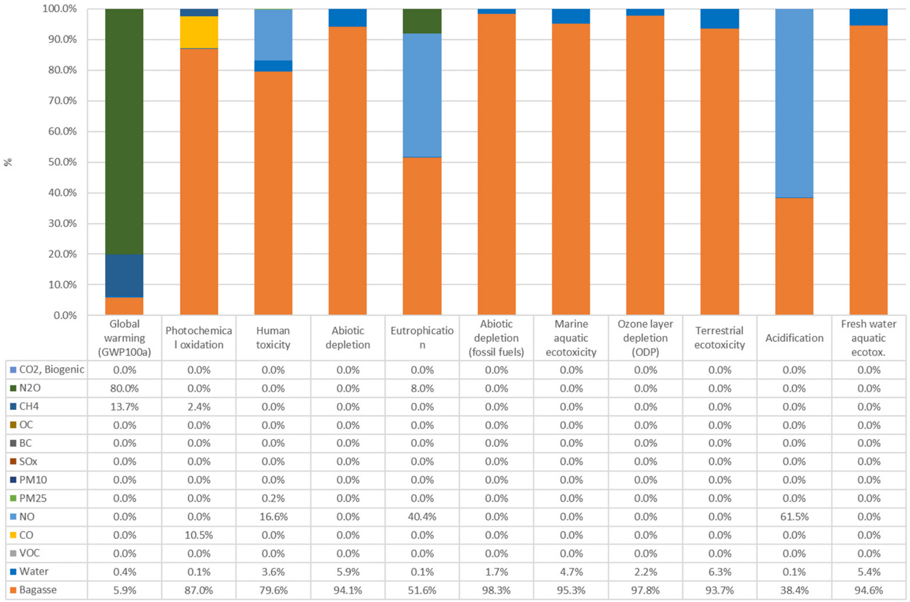
The carbon intensity found for the first and second scenarios are equivalent to 7.99 kg of $CO_2$-eq per MWh and 15.54 kg of $CO_2$-eq per MWh, respectively. This value is equivalent to a reduction of 96% and 92% of the impact of the Brazilian electricity mix that is, according to EcoInvent 3.8 [22], 201.01 kg of $CO_2$-eq per MWh. As shown in the results, the first scenario has lower carbon intensity as it burns the amount of bagasse needed for the required steam production, and the second scenario burns all available bagasse to produce the maximum amount of electricity.

In relation to the economic aspect, the net revenue obtained for the first scenario is USD 2.71 per GJ of steam and surplus electricity, and USD 4.86 per GJ of steam and electricity for the second scenario without any carbon credit. The net revenue was also greater in the second scenario due the higher quantity of electricity sold to the grid; thus, this type of design could be economically interesting.

**Table 6.** LCA results for CHP biomass unit (functional unit: 1 MJ of 2.5 bar steam).

| Impact Categories | Unit | Scenario 1 | Scenario 2 | Δ% |
|---|---|---|---|---|
| Global warming (GWP 100a) | kg $CO_2$-eq/MJ | $2.221 \cdot 10^{-3}$ | $4.317 \cdot 10^{-3}$ | 94% |
| Photochemical oxidation | kg $C_2H_4$-eq/MJ | $2.759 \cdot 10^{-6}$ | $5.125 \cdot 10^{-6}$ | 86% |
| Human toxicity | kg 1,4-DB-eq/MJ | $5.112 \cdot 10^{-4}$ | $1.510 \cdot 10^{-3}$ | 195% |
| Abiotic depletion | kg Sb-eq/MJ | $7.155 \cdot 10^{-9}$ | $2.629 \cdot 10^{-8}$ | 267% |
| Eutrophication | kg $PO_4$-eq/MJ | $2.272 \cdot 10^{-5}$ | $4.182 \cdot 10^{-5}$ | 84% |
| Abiotic depletion (fossil fuels) | MJ/MJ | $5.881 \cdot 10^{-3}$ | $1.378 \cdot 10^{-2}$ | 134% |
| Marine aquatic ecotoxicity | kg 1,4-DB-eq/MJ | $4.399 \cdot 10^{-1}$ | 1.453 | 230% |
| Ozone layer depletion (ODP) | kg CFC-11-eq/MJ | $3.500 \cdot 10^{-11}$ | $8.786 \cdot 10^{-11}$ | 151% |
| Terrestrial ecotoxicity | kg 1,4-DB-eq/MJ | $1.925 \cdot 10^{-6}$ | $7.324 \cdot 10^{-6}$ | 281% |
| Acidification | kg $SO_2$-eq/MJ | $5.731 \cdot 10^{-5}$ | $1.060 \cdot 10^{-4}$ | 85% |
| Fresh water aquatic ecotox. | kg 1,4-DB-eq/MJ | $2.373 \cdot 10^{-4}$ | $8.324 \cdot 10^{-4}$ | 251% |

The EMSO_OLCA tool also allows the user to visualize the contributions of the inputs and the emissions on the LCA category results. Figure 5 illustrates the contribution of inputs and emissions for the LCA of Scenario 1.



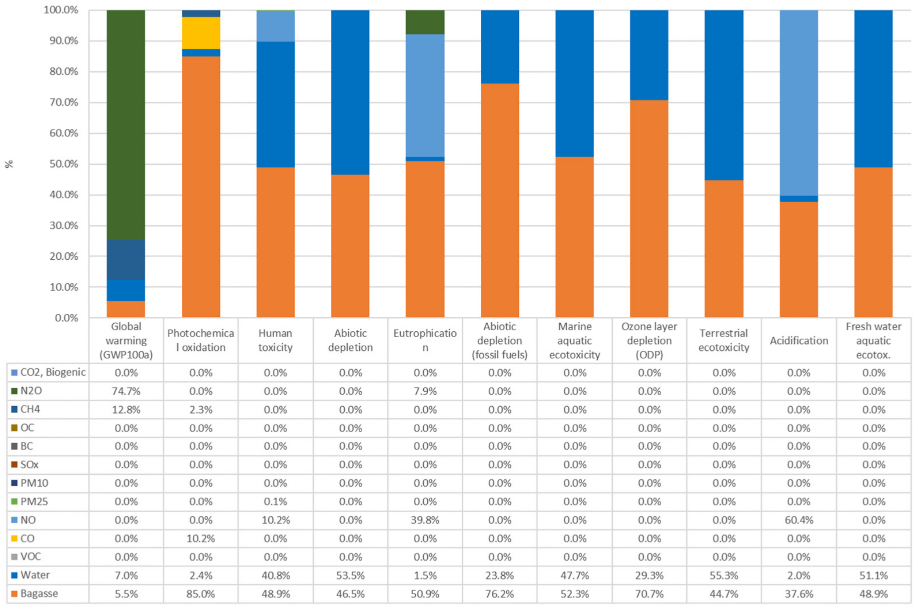
| | Global warming (GWP100a) | Photochemical oxidation | Human toxicity | Abiotic depletion | Eutrophication | Abiotic depletion (fossil fuels) | Marine aquatic ecotoxicity | Ozone layer depletion (ODP) | Terrestrial ecotoxicity | Acidification | Fresh water aquatic ecotox. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ■ CO2, Biogenic | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ N2O | 80.0% | 0.0% | 0.0% | 0.0% | 8.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ CH4 | 13.7% | 2.4% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ OC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ BC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ SOx | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ PM10 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ PM25 | 0.0% | 0.0% | 0.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ NO | 0.0% | 0.0% | 16.6% | 0.0% | 40.4% | 0.0% | 0.0% | 0.0% | 0.0% | 61.5% | 0.0% |
| ■ CO | 0.0% | 10.5% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ VOC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ Water | 0.4% | 0.1% | 3.6% | 5.9% | 0.1% | 1.7% | 4.7% | 2.2% | 6.3% | 0.1% | 5.4% |
| ■ Bagasse | 5.9% | 87.0% | 79.6% | 94.1% | 51.6% | 98.3% | 95.3% | 97.8% | 93.7% | 38.4% | 94.6% |

**Figure 5.** Contribution of the inputs and emissions on the LCA results for Scenario 1.

Figure 5 shows that the bagasse production impact is responsible for most of the impact of the assessed categories except acidification, eutrophication, and global warming. In acidification, the NO produced during bagasse burning is responsible for 61.5% of the impact. In eutrophication, the NO is also responsible for 40.4% of the impact, and in global warming, the dinitrogen oxide also produced during bagasse burning is responsible for 80.0% of the impact of global warming under a horizon of 100 years (GWP 100a).

Figure 6 illustrates the contribution of inputs and emissions for the LCA of Scenario 2.

As shown in Figure 6, the impact of the water increases remarkably in comparison to Figure 5. In this case, the extra steam produced goes to the condensing turbine and needs to be condensed by a cooling tower; thus, the water consumption is increased for the cooling tower water makeup. In relation to eutrophication and acidification categories, they are still impacted by nitrogen oxide emissions, and global warming by the dinitrogen oxide produced during sugarcane bagasse burning.



| | Global warming (GWP100a) | Photochemical oxidation | Human toxicity | Abiotic depletion | Eutrophication | Abiotic depletion (fossil fuels) | Marine aquatic ecotoxicity | Ozone layer depletion (ODP) | Terrestrial ecotoxicity | Acidification | Fresh water aquatic ecotox. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ■ CO2, Biogenic | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ N2O | 74.7% | 0.0% | 0.0% | 0.0% | 7.9% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ CH4 | 12.8% | 2.3% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ OC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ BC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ SOx | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ PM10 | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ PM25 | 0.0% | 0.0% | 0.1% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ NO | 0.0% | 0.0% | 10.2% | 0.0% | 39.8% | 0.0% | 0.0% | 0.0% | 0.0% | 60.4% | 0.0% |
| ■ CO | 0.0% | 10.2% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ VOC | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% | 0.0% |
| ■ Water | 7.0% | 2.4% | 40.8% | 53.5% | 1.5% | 23.8% | 47.7% | 29.3% | 55.3% | 2.0% | 51.1% |
| ■ Bagasse | 5.5% | 85.0% | 48.9% | 46.5% | 50.9% | 76.2% | 52.3% | 70.7% | 44.7% | 37.6% | 48.9% |

**Figure 6.** Contribution of the inputs and emissions on the LCA results for Scenario 2.

As mentioned, a sensitivity analysis can be performed internally in EMSO, showing the variation in the LCA results in relation to process inputs. In order to illustrate this, a sensitivity analysis was conducted of the variation in the 2.5 bar steam consumption in relation to the GWP 100a and net revenue. This sensitivity analysis combined two bagasse prices ranges: USD 14.58 per ton for low bagasse prices and USD 158.75 per ton for high bagasse prices. Figure 7 shows the behavior of GWP 100a and net revenue in the low bagasse price (USD 14.58) scenario according to the steam consumption.

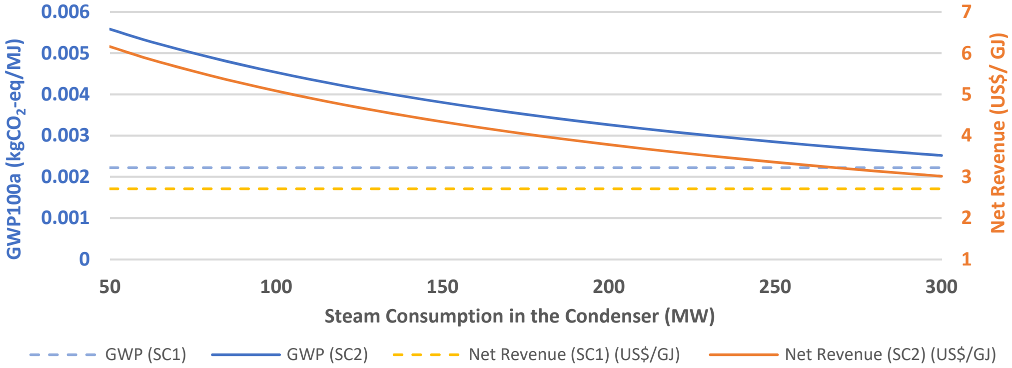


**Figure 7.** Sensitivity analysis of GWP 100a and net revenue for USD 14.58 per ton bagasse price.

In Figure 7, it is evident that in the first scenario (SC1), where the condensing turbine is not present, the carbon intensity remains constant throughout the life cycle regardless of steam consumption. Similarly, the net revenue also remains constant. This observation can be attributed to the adjustment of bagasse and straw burning to meet steam consumption requirements, resulting in a constant carbon intensity and net revenue per GJ of steam and electricity.

The second scenario (SC2) is intriguing as it involves burning all available bagasse and straw to maximize electricity production. The inclusion of a condensing turbine enables greater electricity generation. However, in the studied case, the steam from the condensing turbine is not utilized in the process and is, instead, lost in a cooling tower. Consequently, as electricity production increases, the steam consumption in the condenser decreases, leading to process inefficiency, higher carbon intensity, and increased process net revenue. The net revenue per GJ also rises as more electricity is generated using the same amount of bagasse and straw. This second scenario exemplifies a situation which economic objectives conflict with environmental objectives. Such problems can be further explored in the context of multi-objective optimization.

The same type of sensitivity analysis was also conducted for the higher bagasse price (USD 158.75 per ton), as illustrated in Figure 8.

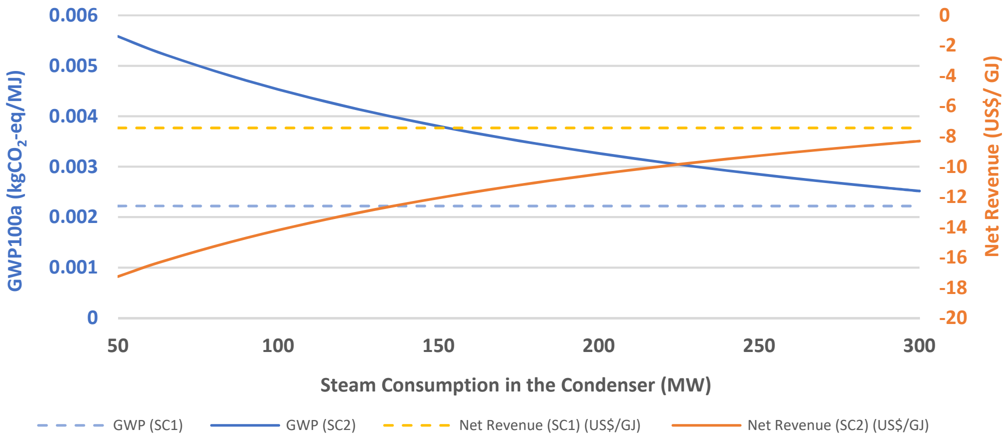


**Figure 8.** Sensitivity analysis of GWP 100a and net revenue for USD 158.75 per ton bagasse price.

According to Figure 8, in Scenario 1 (SC1), it can be observed that the carbon intensity measured by the GWP 100a remains constant regardless of the steam requirement change. This occurs because, as the steam demand increases in this scenario, there is an increase in the combustion of bagasse and straw. This is also reflected in the net revenue, which remains constant.

In Scenario 2 (SC2), with the condensing turbine, the economic results improve as the consumption of steam increases. This case reflects the fact that the price of the electricity does not cover the cost of the fuel. In this case, the carbon intensity of the steam and electricity production is reduced when the steam consumption is increased (only when using cooling towers with a condensing turbine). In this case, both economic and environmental objectives vary in the same direction.

## 4. Conclusions

In this work, a platform named EMSO_OLCA was developed for integrating the open-source software OpenLCA with the open Environment for Modeling, Simulation, and Process Optimization (EMSO) in order to fill the gap between process simulation environments and life cycle assessment software.

EMSO_OLCA allows the user to maintain the consistency of the LCA methodology, as designed in the OpenLCA, and utilize the annually updated LCA databases provided by OpenLCA. EMSO_OLCA provides the computational speed required in simulation software as input calculations was accomplished previously. Another advantage is the integrated tools of EMSO as optimization, sensitivity analysis, and communication to Python, Matlab® and OPC®. The tests demonstrated the accuracy of EMSO_OLCA with a mean relative error of 0.045%.

A cogeneration heat power system with sugarcane bagasse and straw as fuel was studied as a process simulation application. The results for this case study were obtained in just 2.0 s through the integration of EMSO_OLCA. The first scenario presented lower carbon intensity and lower economic results in relation to the second scenario for the bagasse price of USD 14.58. The second scenario with a lower bagasse price (USD 14.58) presented conflicting economic and environmental objectives, and the higher bagasse price

(USD 158.75) presented environmental and economic objectives in the same direction as varying steam requirements. Thus, the price of the raw materials could influence whether the economic and environmental objectives are conflicting or not.

The studied sugarcane bagasse heat and power units allow a significant reduction in the carbon footprint compared to the Brazilian electricity grid, representing 96% and 92% for the first scenario and the second scenario, respectively. The first and second scenarios achieved a GWP 100a of 7.99 and 15.54 kg of $CO_2$-eq per MWh, in contrast to the Brazilian mix of 201.01 kg of $CO_2$-eq per MWh. Thus, biomass-based cogeneration units should be promoted by governmental policies and financing agencies.

EMSO_OLCA has been shown to be a powerful tool to enhance the decision-making process allied to process simulation when evaluating different chemical pathways; it facilitates comprehensive techno-economic and environmental assessments, and empowers the optimization and control of processes based on environmental performance indicators.

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**Data Availability Statement:** The computational files are available from https://github.com/LADES-PEQ/EMSO_OLCA (accessed on 12 June 2024).

**Conflicts of Interest:** The authors declare no conflicts of interest.

## References

1. *ISO 14040*; Environmental Management—Life Cycle Assessment—Principles and Framework. International Standard Organization: Geneva, Switzerland, 2006. Available online: https://www.iso.org/standard/37456.html (accessed on 1 January 2022).
2. OpenLCA. Available online: https://www.openlca.org/ (accessed on 1 January 2022).
3. Simapro. Available online: https://simapro.com/ (accessed on 1 January 2022).
4. LCA for Experts. Available online: https://sphera.com/solutions/product-stewardship/life-cycle-assessment-software-and-data/lca-for-experts/ (accessed on 12 June 2024).
5. Potrich, E.; Miyoshi, S.C.; Machado, P.F.S.; Furlan, F.F.; Ribeiro, M.P.A.; Tardioli, P.W.; Giordano, R.L.C.; Cruz, A.J.G.; Giordano, R.C. Replacing hexane by ethanol for soybean oil extraction: Modeling, simulation, and techno-economic-environmental analysis. *J. Clean. Prod.* **2020**, *244*, 118660. [CrossRef]
6. Carpio, R.R.; Miyoshi, S.C.; Elias, A.M.; Furlan, F.F.; Giordano, R.C.; Secchi, A.R. Multi-objective optimization of a 1G-2G biorefinery: A tool towards economic and environmental viability. *J. Clean. Prod.* **2021**, *284*, 125431. [CrossRef]
7. Ferdous, J.; Bensebaa, F.; Pelletier, N. Integration of LCA, TEA, Process Simulation and Optimization: A systematic review of current practices and scope to propose a framework for pulse processing pathways. *J. Clean. Prod.* **2023**, *402*, 136804. [CrossRef]
8. Kalakul, S.; Pomthong, M.; Kitipat, S.; Rafiqul, G. Integration of life cycle assessment software with tools for economic and sustainability analyses and process simulation for sustainable process design. *J. Clean. Prod.* **2014**, *71*, 98–109. [CrossRef]
9. Guinée, J.B.; Gorrée, M.; Heijungs, R.; Huppes, G.; Kleijn, R.; de Koning, A.; van Oers, L.; Wegener Sleeswijk, A.; Suh, S.; Udo de Haes, H.A.; et al. Handbook on life cycle assessment. In *Operational Guide to the ISO Standards. I: LCA in Perspective. IIa: Guide. IIb: Operational Annex. III: Scientific Background*; Kluwer Academic Publishers: Dordrecht, The Nederland, 2002; p. 692. ISBN 1-4020-0228-9. [CrossRef]
10. Huijbregts, M.A.J.; Steinmann, Z.J.N.; Elshout, P.M.F.; Stam, G.; Verones, F.; Vieira, M.; Zijp, M.; Hollander, A.; Zelm, R.V. ReCiPe2016: A harmonized life cycle impact assessment method at midpoint and endpoint level. *Int. J. Life Cycle Assess.* **2017**, *22*, 138–147. [CrossRef]
11. Soares, R.P.; Secchi, A.R. EMSO: A New Environment for Modelling, Simulation and Optimisation. *Comput. Aided Chem. Eng.* **2003**, *14*, 947–952. [CrossRef]
12. OPC. Available online: https://opcfoundation.org/ (accessed on 12 June 2024).
13. Python 3.0. Available online: https://www.python.org/download/releases/3.0/ (accessed on 12 June 2024).
14. Matlab. Available online: https://www.mathworks.com/products/matlab.html (accessed on 12 June 2024).
15. Scilab. Available online: https://www.scilab.org/ (accessed on 12 June 2024).
16. Excel. Available online: https://www.microsoft.com/pt-br/microsoft-365/excel (accessed on 12 June 2024).

17. LibreOffice. Available online: https://www.libreoffice.org/discover/libreoffice/ (accessed on 12 June 2024).
18. *ISO 14044*; Environmental Management—Life Cycle Assessment—Requirements and Guidelines. International Standard Organization: Geneva, Switzerland, 2006. Available online: https://www.iso.org/standard/38498.html (accessed on 1 January 2022).
19. Jolliet, O.; Saadé, M.; Crettaz, P. *Analyse du Cycle de Vie: Comprendre et Réaliser un Écobilan*; PPUR Presses Polytechniques: Geneva, Switzerland, 2010; Volume 23.
20. Agarwal, N.K.; Kumar, M.; Pattnaik, F.; Kumari, P.; Vijay, V.K.; Kumar, V. Exploring the Valorization Potential of Sugarcane Bagasse Pith: A Review. *BioEnergy Res.* **2023**, *16*, 1280–1295. [CrossRef]
21. Ungureanu, N.; Vlăduț, V.; Biriș, S.Ș. Sustainable valorization of waste and by-products from sugarcane processing. *Sustainability* **2022**, *14*, 11089. [CrossRef]
22. Wernet, G.; Bauer, C.; Steubing, B.; Reinhard, J.; Moreno-Ruiz, E.; Weidema, B. The ecoinvent database version 3 (part I): Overview and methodology. *Int. J. Life Cycle Assess.* **2016**, *21*, 1218–1230. [CrossRef]
23. CML-IA 2016. Available online: https://www.universiteitleiden.nl/en/research/research-output/science/cml-ia-characterisation-factors (accessed on 1 January 2022).
24. Rocha, G.J.M.; Nascimento, V.M.; Goncalves, A.R.; Silva, V.F.N.; Martín, C. Influence of mixed sugarcane bagasse samples evaluated by elemental and physical–chemical composition. *Ind. Crops Prod.* **2015**, *64*, 52–58. [CrossRef]
25. Bonomi, A.; Mariano, A.P.; Jesus, C.D.F.; Franco, H.C.J.; Cunha, M.P.; Dias, M.O.S.; Chagas, M.F.; Cavalett, O.; Mantelatto, P.E.; Maciel Filho, R.; et al. *The Virtual Sugarcane Biorefinery (VSB)*; Technological Assessment Program (PAT), Internal Report; Brazilian Bioethanol Science and Technology Laboratory (CTBE): Campinas/São Paulo, Brazil, 2012.
26. Oliveira, R.A.; Barros, R.R.O.; Ferreira-Leitão, V.S.; Freitas, S.P.; Bon, E.P.S. Energy supply design for the integrated production of 1G + 2G ethanol from sugarcane. *Renew. Energy Focus.* **2020**, *35*, 171–177. [CrossRef]
27. Dias, M.O.S. Development and Optimization of First and Second Generation Ethanol and Electricity Production Processes from Sugar Cane. Ph.D. Thesis, Chemical Engineering Faculty, Universidade Estadual de Campinas, Campinas, Brazil, 2011. (In Portuguese).
28. Dias, M.O.; Junqueira, T.L.; Cavalett, O.; Cunha, M.P.; Jesus, C.D.; Mantelatto, P.E.; Rossel, C.E.V.; Maciel Filho, R.; Bonomi, A. Cogeneration in integrated first and second generation ethanol from sugarcane. *Chem. Eng. Res. Des.* **2013**, *91*, 1411–1417. [CrossRef]
29. Furlan, F.F.; Filho, R.T.; Pinto, F.H.; Costa, C.B.; Cruz, A.J.; Giordano, R.L.; Giordano, R.C. Bioelectricity versus bioethanol from sugarcane bagasse: Is it worth being flexible? *Biotechnol. Biofuels* **2013**, *6*, 142. [CrossRef]
30. Wang, M.; Elgowainy, A.; Lu, Z.; Bafana, A.; Benavides, P.; Burnham, A.; Cai, H.; Dai, Q.; Gracida, U.; Hawkins, T.; et al. *Greenhouse Gases, Regulated Emissions, and Energy Use in Technologies Model® (2020.Net)*; Argonne National Laboratory (ANL): Argonne, IL, USA, 2020. [CrossRef]
31. CEDAE. Tariff Structure. 2022. Available online: https://cedae.com.br/estruturatarifaria (accessed on 15 May 2024). (In Portuguese).
32. Águas do Rio. Legislation and Tariffs. 2023. Available online: https://aguasdorio.com.br/legislacao-e-tarifas/ (accessed on 15 May 2024). (In Portuguese).
33. ANEEL. National Electric Energy Agency. 2023. Available online: https://www.gov.br/aneel/pt-br (accessed on 15 May 2024). (In Portuguese)
34. MDIC. Ministry of Development, Industry, Commerce and Services COMEXSTAT. 2023. Available online: http://comexstat.mdic.gov.br/pt/home (accessed on 1 January 2023).