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Life Cycle Analysis of Succinic Acid Production in the Brazilian Biorefinery Context

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Abstract: Succinic acid is an essential component of the chemical industry. Traditionally produced from fossil resources, its sustainable production using renewable resources faces challenges due to the complexities of cultivation and purification. This study assessed the environmental impacts of succinic acid production from sugarcane through a life cycle analysis and compared it with three other scenarios: using sorghum, apple pomace, and the traditional chemical route. Employing the ReCiPe midpoint methodology with a cradle-to-gate approach, the analysis highlighted significant environmental impacts linked to the agricultural stage in the sugarcane process. The use of pesticides, fertilizers, and energy demand resulted in elevated impacts compared to other stages of the process. The other scenarios also presented strong contributions in the purification stages. The production from sugarcane proved advantageous compared to other scenarios, minimizing impacts in 6 out of 10 categories. It is evident that the selection of the correct biomass is crucial for process sustainability, and the use of second-generation inputs can help reduce impacts in the agricultural stage. However, advancements in the fermentation stage are necessary, along with a reduction in the complexity of the purification steps. This study emphasizes the potential of renewable succinic acid production from sugarcane juice in the Brazilian scenario. Utilizing this process could reduce succinic acid's environmental impacts by 70% to 99% compared to the petrochemical route. The process should be considered as a sustainable alternative to be included in the portfolio of biorefineries, enhancing factory profitability.

Keywords: bio-based succinic acid; fossil-based succinic acid; life cycle assessment



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1. Introduction

The search for processes based on renewable resources is of great interest to industry given environmental issues such as climate change and energy security. Currently, the global chemical industry, a sector responsible for the production of intermediate and final products, and which is essential to the modern global economy, is heavily dependent on non-renewable resources, either as a source of raw materials or energy. Therefore, the increasing global demand for chemicals, driven largely by technological advances, as well as population and economic growth, has put a strain on fossil resources. According to the International Energy Agency, crude oil and natural gas represent more than 80% of the feedstocks in the carbon-based chemical industry [1]. Within the chemical industry, organic acids have great applicability, with emphasis on carboxylic acids, which are oxygen-rich and highly reactive molecules that have a wide range of applications in the production of

important products in the food, pharmaceutical, cosmetic, and textile industries, among others [2,3].

Succinic acid (SA) is a saturated dicarboxylic acid that can be produced biochemically, as the main product of anaerobic fermentation in some microorganisms, or produced as an intermediate of the tricarboxylic acid cycle [4]. The compound is considered one of the 20 building blocks, presenting numerous applications in the chemical, food, pharmaceutical, and cosmetic industries [5], while also acting as an intermediate for the production of various polymers, resins, and plasticizers [6]. In 2021, the market value of SA was USD 160.8 million, with a forecast of USD 301.4 million by 2032, showing a growth of 6.5% per year [7]. Most of its production is currently carried out by a chemical route based on the catalytic hydrogenation of maleic anhydride, a fossil compound derived from benzene or n-butane [8].

There are already processes implemented by companies such as Myriant, Bioamber, Reverdia, and Succinity that use the biotechnological route to produce SA, using glucose or glycerol as a carbon source for microorganisms. However, the small-scale production is related to the higher price of renewable SA compared to fossil SA [9], which limits its competitiveness [10]. According to Dickson et al. [9], the main difficulties are in the downstream steps, since the SA intended as a raw material for polymer production requires a high purity.

In the Brazilian scenario, the association of SA production with the sugar and ethanol industry may be a strategic alternative, since the country accounts for 37% of the world's sugarcane production [11], besides having a robust and well-developed sugarcane-based sector. The processes described by Efe et al. [12] allow for the conversion of sugarcane sucrose into SA, which allows for the integration of the process into ethanol distilleries, increasing the product portfolio of the plant. Including value-added products in a biorefinery's portfolio can help make it economically feasible, as it contributes significantly to the plant's profitability [13].

Despite the benefits associated with eliminating the use of fossil resources, the biotechnological routes face environmental issues due to the impacts associated with the agricultural phase and the use of energy and several chemicals in their purification processes, which are more complex compared to the chemical route. Smidt et al. [6] conducted a Life Cycle Assessment (LCA) of SA production from corn and found increased dust and particulate matter emissions. Cok et al. [8] compared different routes (low pH fermentation, anaerobic fermentation, and a chemical route from maleic anhydride) and found that low pH fermentation followed by direct crystallization resulted in lower environmental impacts. Conversely, the work of González-García et al. [14] highlighted significant impacts in the extraction and distillation steps. Brunklaus et al. [15] contributed by identifying the environmental benefits of using food waste as a substrate over virgin biomass, as observed in the case of corn. Together with studies by Gadkari [10], Ioannidou [16], Foulet [17], and Khoshnevisan [18], these works provide a comprehensive basis for understanding the environmental and economic impacts of different waste sources in the context of SA production.

Among the studies already carried out on the environmental performance of SA production processes, there is a lack of data on its production from sugarcane with the aim of SA integration in biorefineries. Other carbon sources have produced good results, but within the Brazilian context, sugarcane can be an ally in minimizing impacts, considering already well-established mills. In this context, this study analyzed the environmental impacts associated with the production of SA from sugarcane within the Brazilian scenario, seeking to identify possible trade-offs compared to other alternative routes for the production of SA from renewable sources, such as the process used by Myriant using sorghum as feedstock, a second-generation (2G) process using lignocellulosic biomass waste and the conventional chemical route.

2. Materials and Methods

The environmental performance of SA production, from biochemical and chemical routes, was evaluated using LCA based on ISO 14040 [19] and ISO 14044 [20] guidelines. The modeling was performed in SimaPRO® 9.2.0. Additional assumptions are described as follows.

2.1. Scope Definition

The cradle-to-gate approach was considered, since there is no expected difference in the life cycle of the SA transport, distribution, and use steps for the considered scenarios. Impacts related to the agricultural step were embedded in the upstream step.

To compare the environmental impacts of the SA production from sugarcane (1st scenario), three other scenarios were selected based on works from the literature but adapted to the Brazilian scenario through inventories of energy use and inputs to the country's reality. These are as follows: 2nd scenario—the first-generation biochemical route from sorghum; 3rd scenario—the second-generation (2G) process using apple waste proposed by González-García et al. [14]; and the 4th scenario—the chemical route from maleic anhydride (Figure 1). All scenarios, which are described in detail in Section 2.2, were considered for their operation in the Brazilian territory to establish a fair comparison between the four alternatives.

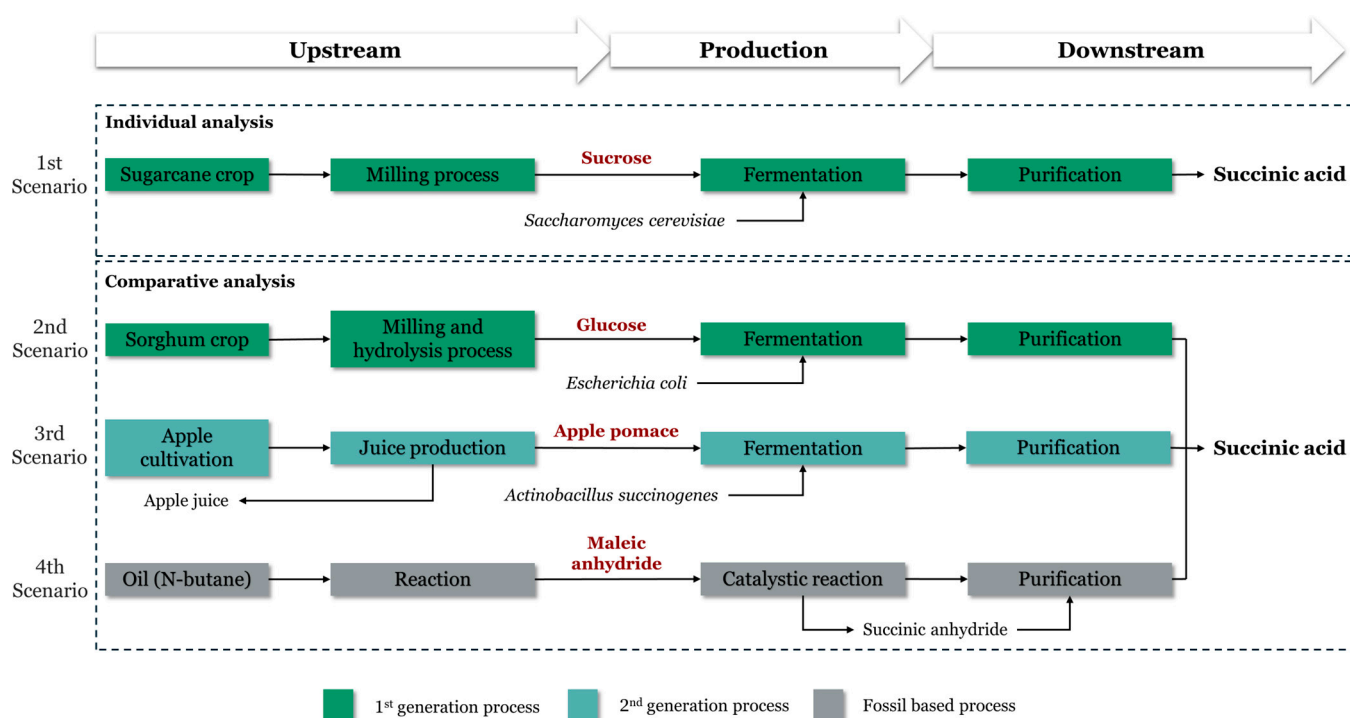


Figure 1. Scope and stages of the four scenarios of succinic acid production considered in the LCA study.

The selection of raw materials in this study was grounded in the combination of national input availability and data accessibility in the literature. The 1st scenario employs sugarcane as a raw material cultivated in Brazil, the world's largest producer with 724 million tons in 2022 [21]. In addition to the abundant supply of sugarcane, the country boasts a robust and extensive sugar and alcohol industry. This enables the integration of succinic acid production into existing mills. Integrated production facilitates the utilization of electricity and heat generated by burning sugarcane bagasse, contributing significantly to the sustainability of the process. The 2nd scenario was modeled after the Myriant process, which is a consolidated and industrial process using sorghum as the raw material. Sorghum cultivation boasted an annual production of 2.92 million tons in 2022 [22], emphasizing

its availability, particularly in the central-western region of the country. The 3rd scenario involves the utilization of apple pomace as the raw material. Brazil's annual apple production is noteworthy, reaching approximately 1.05 million tons cultivated across around 33 thousand hectares, primarily concentrated in the southern and southeastern regions [23]. Apple juice finds extensive use in the beverage industry, serving as a natural sweetener in nectars and other fruit drinks, replacing part of the sugar that would otherwise be added to the product. This results in significant fruit consumption, both in its natural form and as juice. However, apple juice production generates a significant byproduct, apple pomace, which can be used for succinic acid production, as stated by Gonzalez-Garcia [14]. The 4th scenario, the chemical route, involves the use of maleic anhydride for SA production. The maleic anhydride is produced in Brazil with a capacity of 30 thousand metric tons per year [24], and the main suppliers are located in the southeastern region of the country.

Since this is a comparative analysis of the production step, the functional unit was defined as 1 kg of SA produced with a purity index higher than 99.5% in all scenarios analyzed. The 2nd scenario, which uses sorghum, produces 1.49 kg of ammonium sulfate (AMS) per 1 kg of SA. Since this is a product widely used as fertilizer, the AMS produced can be a direct substitute for petrochemical AMS and, like SA, presents a sustainable appeal for its consumption.

2.2. Scenarios Description

2.2.1. The 1st Scenario (Reference Scenario): SA from Sugarcane

The studies by Efe et al. [12] and Furlan [25] addressed the production of SA using the 1G process in the Brazilian context, using a biotechnological route based on the fermentation of sucrose from sugarcane juice by *Saccharomyces cerevisiae*, considering the whole production process, and performing technical-economic simulations. The study conducted by Efe et al. [12] addressed the production of SA via a biotechnological route using recombinant *S. cerevisiae* and a purification process using adsorption with zeolites. The process is on an industrial scale with an SA production capacity of 30 thousand tons per year. The study by Furlan [25] performed a reverse techno-economic analysis. The process was simulated in EMSO 0.10.11 software, where it was modeled from the mass and energy balances of all the equipment involved from the sugarcane juice sterilization stage to the rotary filtration stage, according to the flowchart shown in Figure 2.

The sugarcane plantation inventory was taken from the Ecoinvent 3 database. The juice extraction stage was taken from the study carried out by Ocampo Battle [26]. The industrial process starts with the passage of the sugarcane juice added to a recycle stream through a sterilizer, where the temperature is raised to 134 °C and then reduced to 30 °C. The stream is directed to the fermenter, where the microorganism *S. cerevisiae* is used, because of its robustness at a lower pH. The fermentation is carried out at 30 °C and a pH close to 4, aiming at a final SA concentration of 13.7 g/L. After fermentation, the wort is sent to a centrifugation step for cell recovery, which is recycled to the fermenter. The cell-free stream is passed to an adsorption column step. During the desorption step, water at 150 °C is used as a desorption stream, and the output is directed to a flash evaporator to remove excess water. After evaporation, the stream is directed to a storage tank to ensure process continuity for the next steps, which consist of an evaporation step, followed by crystallization. The resulting crystals are separated with a rotary drum filter and dried in a rotary dryer. During the adsorption process, ZSM-5 zeolite is used, and calcination steps are required every 3 production cycles to recover its properties. The zeolite is replaced annually.

To establish a comparison of the environmental impacts related to the first-generation (1G) process from sugarcane juice, three other scenarios are elaborated based on data from the literature, but relevant to the Brazilian scenario, by adapting their inventories of energy and inputs used.

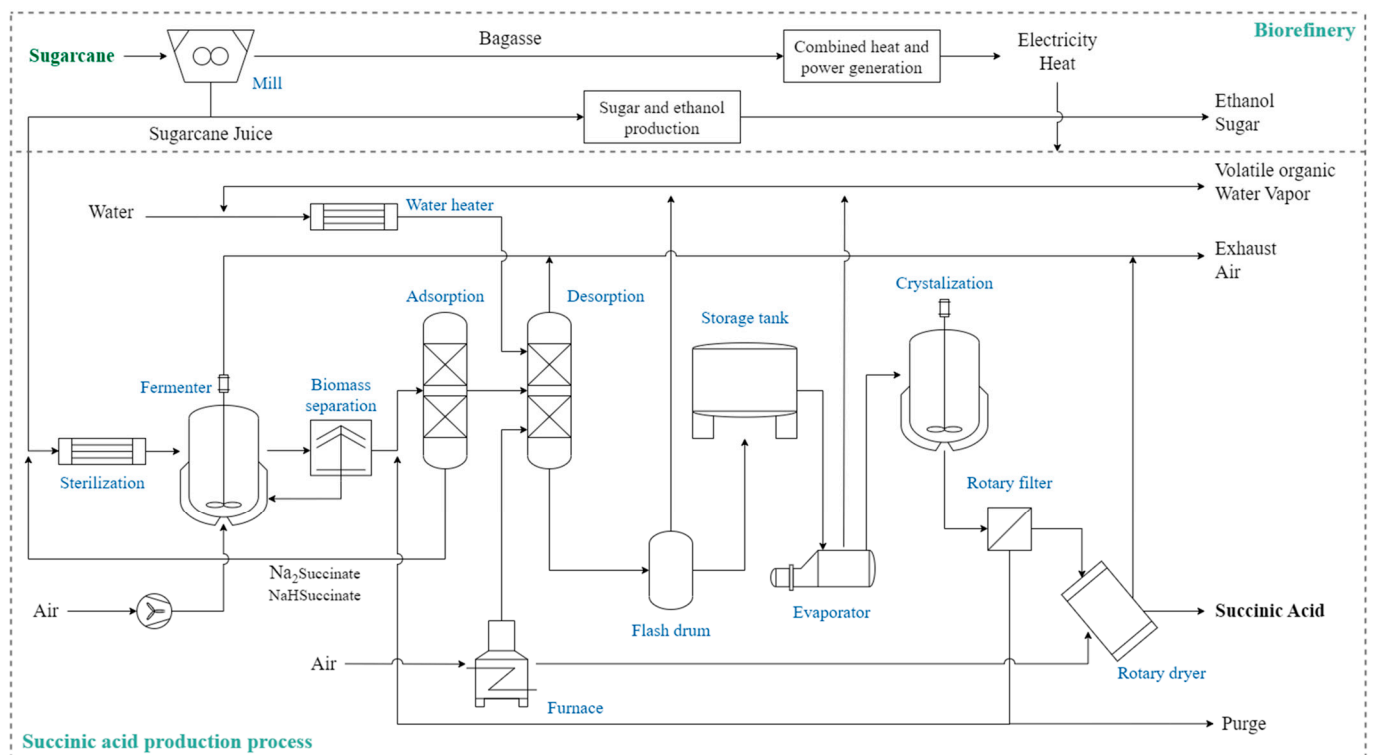


Figure 2. Flowchart of the 1st scenario where succinic acid is produced from sugarcane juice.

2.2.2. The 2nd Scenario: SA Production from Sorghum

The 2nd scenario refers to the industrial process implemented by Myriant Technologies LLC, which uses sorghum as the carbon source and recombinant *Escherichia coli* to produce SA. The purification process includes several stages such as clarification, filtration, ion extraction, evaporation, and crystallization [27]. The process also has a by-product, ammonium phosphate, which is used as a fertilizer for sorghum cultivation, removing the need to apply the allocation since the compound returns to the process. The scenario development was based on Moussa et al. [28], who addressed the energy performance of SA production from biotechnological routes. As this is an implemented process, the data provided by Myriant [27] allowed for the idealization of an inventory for the production process, complemented by the inventory of sorghum cultivation from Donke et al. [29].

2.2.3. The 3rd Scenario: SA Production from Apple Pomace

The 3rd scenario refers to the 2G process proposed by González-García et al. [14], which assumed the use of apple pomace, a waste product from the food industry, as a carbon source for the biotechnological route that uses *Actinobacillus succinogenes* for the SA production. The process uses pretreatments such as drying, followed by fermentation and a complex purification process that includes centrifugation, ultrafiltration, reactive extraction, vacuum distillation, and crystallization, to obtain SA with a purity of more than 99.5%. The study by González-García et al. [14] included an environmental analysis of the process by varying several parameters such as enzyme production, the conditions for SA extraction, and the recovery of organic solvents. The study analyzed Spanish and global inventories using the CML method. For this study, the inventories were brought into the Brazilian perspective by using Brazilian inventories for process inputs.

2.2.4. The 4th Scenario: Conventional Fossil SA Production from Maleic Anhydride

The 4th scenario corresponds to the chemical route of SA production, which was described by Pinazo et al. [30]. The route is based on the catalytic hydrogenation of maleic anhydride, a fossil compound. The process consists of exposing the maleic anhydride in

the liquid phase between 120 and 180 °C at moderate pressures in the presence of catalysts composed of nickel and palladium, forming succinic anhydride. The catalysts are then removed through filtration, followed by distillation. The succinic anhydride is hydrated to SA, which is then filtered and dried [27]. The study of Pinazo et al. [30] is the basis for establishing the chemical route inventory.

2.3. Life Cycle Inventory Data and Sources

All scenarios were adapted to the Brazilian territory using energy from the country's energy matrix, except for the 1st scenario, which uses energy produced in the plant itself. The inputs are preferably produced in Brazil. The inventories cover the agricultural stages of sugarcane and sorghum, the transportation to the processing site, and the production stage, ending with the obtaining of the SA.

The scenarios were strategically positioned across the country to minimize the transportation needs of raw materials, as shown in Figure 3. A production scale of 3000 annual tons of succinic acid was established, which corresponds to approximately 5% of the global demand for the compound [31] and is capable of supplying the entire volume of national imports [32].

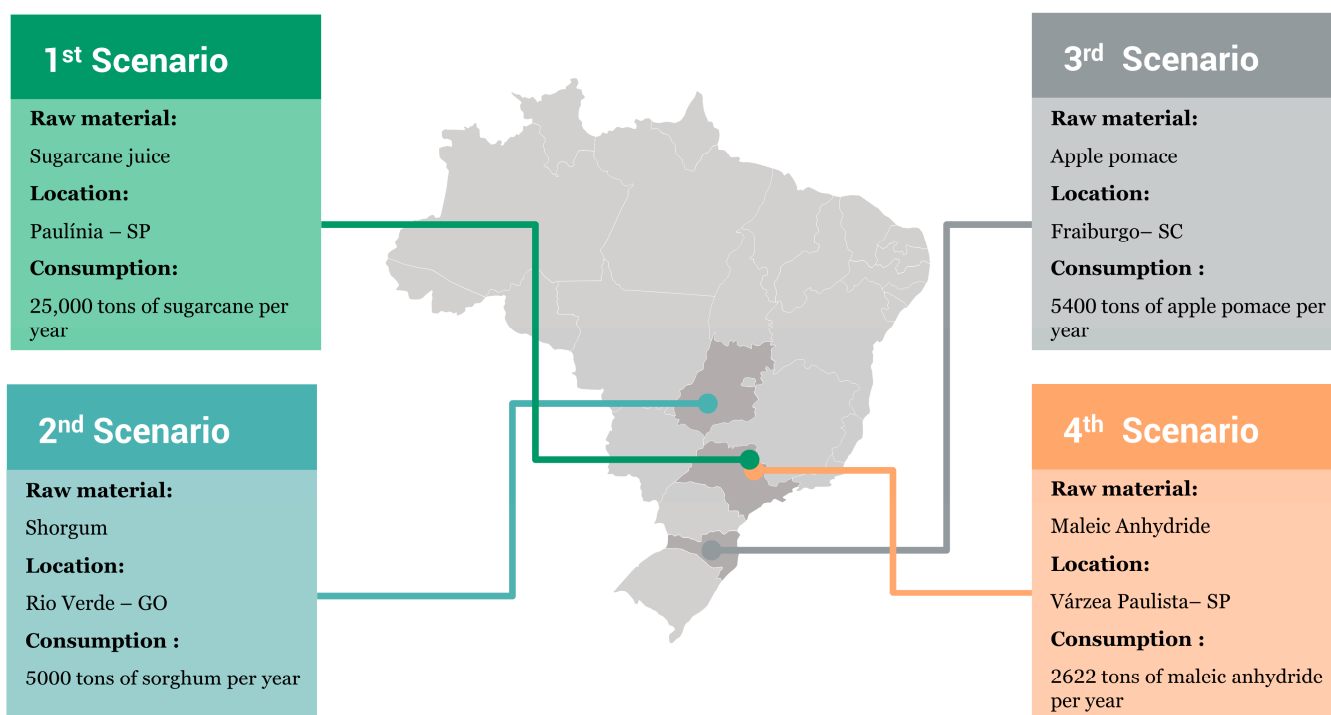


Figure 3. Location of the unit plant for each scenario on the map of Brazil, highlighting the raw materials and their consumption.

The 1st Scenario, related to the 1G process of SA production from sugarcane, considered the sugarcane's agricultural stage in the southeast region of Brazil using the inventory available in the Ecoinvent 3.5 database. The unit location of the process was set in the city of Paulínia in the state of São Paulo. The state has an annual production of 420 million tons of sugarcane [33], which generates sufficient output to supply the process demand within a radius of 30 km. The transportation and milling steps were taken from Ocampo Batlle et al. [26]. The SA production plant is annexed to a sugar and ethanol mill, which is supplied by the bagasse used in a cogeneration system. The inventory related to the production process was taken from the data obtained from the simulation of the process in EMSO software [25]. In order to analyze the 1st Scenario separately, the process was divided into the upstream stage, which takes into account the agricultural stage, trans-

portation, and milling of the sugarcane; the fermentation stage; and the downstream stage where the purification of SA is carried out. This resulted in three different inventories that allowed for the environmental analysis of the impacts associated with each one of them.

The 2nd scenario, which is based on the process developed by Myriant, used the sorghum as a feedstock inventory, taken from Donke et al. [29], with adjustments made in the origin of inputs to bring it into the Brazilian perspective. The plant's location of the process was set in the city of Rio Verde, in the state of Goiás, which has an annual sorghum production of 148,000 tons [34]. This high production output can supply the entire demand for the process with a transportation radius of 30 km. The inventory of the production process, taken from Moussa et al. [28], considers the direct input of sorghum seeds until the SA is obtained. However, the input of sorghum seeds brings with it the impacts associated with its agricultural stage.

The 3rd scenario, the 2G process from apple pomace, disregarded the stages of obtaining apple pomace since it is a residue normally discarded from the apple juice production process. The plant is located in the city of Fraiburgo, in the state of Santa Catarina. The city has an annual production of 55,370 tons of apples [35]. It also has the Fischer factory, the largest producer of apple juice in Brazil, which makes it possible to supply integral raw materials within a radius of 30 km. The inventory, taken from González-García et al. [14], considers apple pomace input to the obtaining of the SA.

The 4th Scenario, the traditional chemical route, used an adaptation of the maleic anhydride inventory available in the Ecoinvent 3.5 database to represent the production of the input in Brazil (see Table S3 in Supplementary Material for more details). According to data from COMEXSTAT [36], the input is produced on a large scale in Brazil and has a low import volume. The process is located in the Várzea Paulista region, a municipality with the highest national production of maleic anhydride, with 30,000 tons per year [24]. The SA production plant operates in conjunction with the maleic anhydride production unit, operated by Elekeiroz, consuming approximately 8.7% of its production and eliminating the need for raw material transportation. The inventory related to the production step was taken from the work of Pinazo et al. [30], considering the addition of maleic anhydride until the obtaining of the SA. The detailed inventory of all scenarios evaluated can be found in the Supplementary Material.

2.4. Life Cycle Impact Assessment Methodology

The ReCiPe methodology [37] was used for environmental assessment considering eleven midpoint categories: individualistic cultural perspectives. These were as follows: AP—acidification potential (kg SO₂ eq); EP—eutrophication potential (kg P eq); GWP—global warming potential (kg CO₂ eq); ODP—ozone depletion potential (kg CFC—11 eq); POP—photochemical oxidation potential (kg NMVOC); HTP—human toxicity potential (kg 1,4-DB eq); AEP—aquatic ecotoxicity potential (kg 1,4-DB eq); TEP—terrestrial ecotoxicity (kg 1,4-DB eq); MD—metal depletion (kg Fe eq); FD—fossil depletion (kg oil eq).

3. Results

3.1. LCA of the SA Integrated into the 1G Biorefinery

The LCA results of the SA from the 1G process integrated into the sugarcane biorefinery (1st scenario) are presented in Figure 4, including the upstream, fermentation, and downstream stages of the SA production (highlighting the percentage contributions of each stage).

Within the analyzed stages, the most substantial contribution comes from the upstream process. This stage encompasses all impacts associated with sugarcane planting, transporting, and processing, and sucrose juice extraction, resulting in consequences across all categories. The agricultural phase is the largest contributor to the environmental burden, and the primary contributions are linked to the use of fertilizers, such as urea, and insecticides, contributing to mineral resource depletion and terrestrial acidification. Additionally, the diesel used in transportation contributes to both global warming potential

and fossil resource scarcity. The large effect on the environmental impacts of the traditional sugarcane biorefineries occurs in the agricultural stage as indicated in literature [38,39].

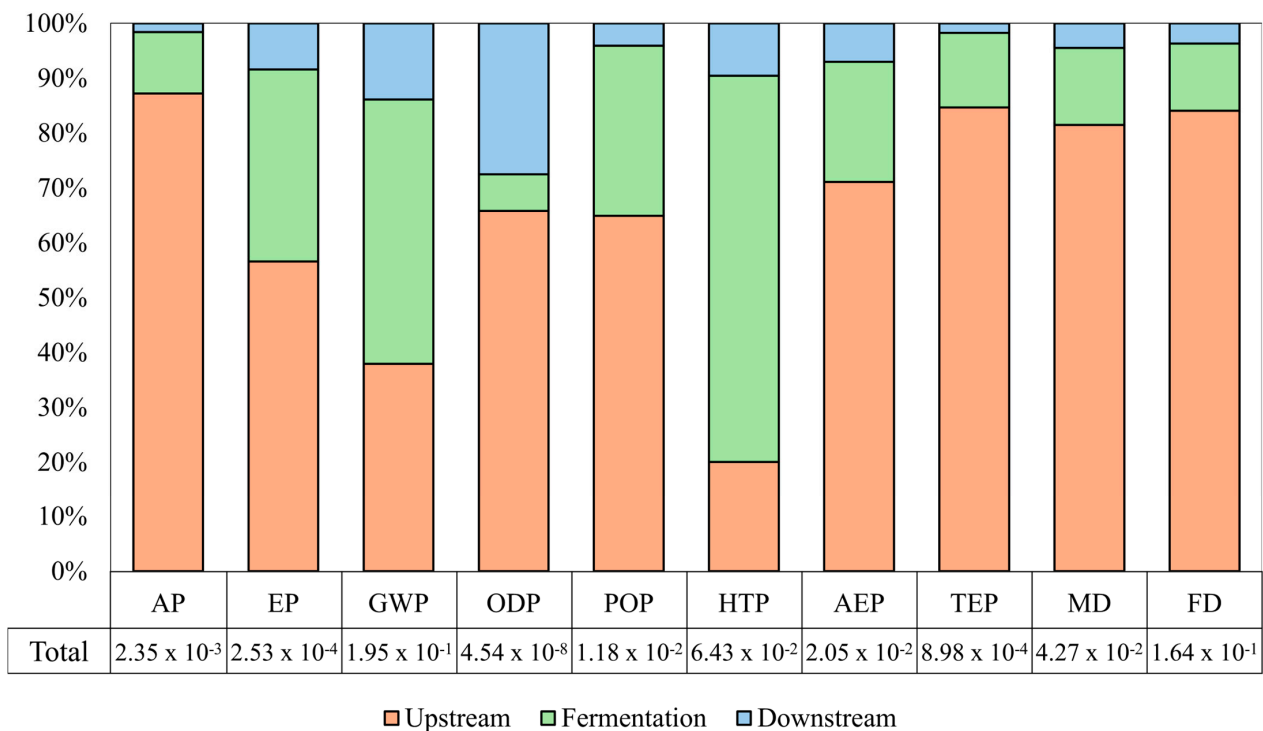


Figure 4. Contribution of each production stage to environmental impacts in the process of producing succinic acid from sugar cane. AP—acidification potential (kg SO₂ eq); EP—eutrophication potential (kg P eq); GWP—global warming potential (kg CO₂ eq); ODP—ozone depletion potential (kg CFC—11 eq); POP—photochemical oxidation potential (kg NMVOC); HTP—human toxicity potential (kg 1,4-DB eq); AEP—aquatic ecotoxicity potential (kg 1,4-DB eq); TEP—terrestrial ecotoxicity (kg 1,4-DB eq); MD—metal depletion (kg Fe eq); FD—fossil depletion (kg oil eq).

In the fermentation stage, the impacts are primarily attributed to electricity and ammonia usage. While the impacts could be higher, all energy utilized is generated onsite through the combustion of bagasse, effectively minimizing and balancing carbon emissions. Nevertheless, fermentation significantly influences subsequent purification steps, involving the production of by-products, compound purity, and the necessity to separate cells from the medium. As a biotechnological process, the fermentation must entail a considerable volume of water, cells, metabolic by-products, and solids from the carbon source, requiring multiple sequential filtration, adsorption, and evaporation steps.

Downstream operations contribute significantly due to the substantial energy demand in SA purification processes. The utilization of NaOH and zeolites further adds to the impacts, stemming from emissions associated with their production (constituting approximately 28% of ozone depletion impacts and 14% of carbon emissions). As highlighted by Efe et al. [12], downstream processes play a pivotal role in operational costs, underscoring their importance for the overall viability of the production process.

3.2. Sensitivity Analysis of the SA Integrated into the 1G Biorefinery

A sensitivity analysis (Figure 5) conducted in the 1st scenario emphasized the significant influence that variations in the fermentation process can exert on the overall process. Two variables were selected for scrutiny: the selectivity of AS relative to ethanol and the specific productivity of the fermentation (grams of SA/kilogram of yeast/hour). A variation of plus and minus 20% was applied to these variables to quantify the impacts associated with

the modified process. Figure 5 illustrates the percentage variation of each impact category in comparison to the base scenario.

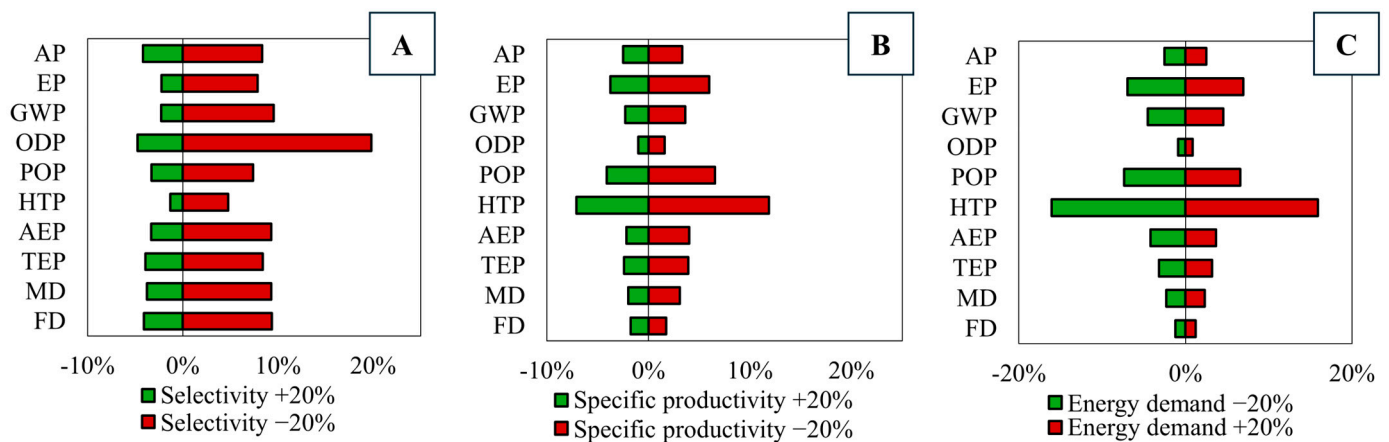


Figure 5. Sensitivity analysis that represents the percentage variation in environmental impacts by varying selectivity (A), specific productivity (B), and energy demand (C) in relation to the base scenario for the production of succinic acid from sugar cane. AP—acidification potential (kg SO₂ eq); EP—eutrophication potential (kg P eq); GWP—global warming potential (kg CO₂ eq); ODP—ozone depletion potential (kg CFC—11 eq); POP—photochemical oxidation potential (kg NMVOC); HTP—human toxicity potential (kg 1,4-DB eq); AEP—aquatic ecotoxicity potential (kg 1,4-DB eq); TEP—terrestrial ecotoxicity (kg 1,4-DB eq); MD—metal depletion (kg Fe eq); FD—fossil depletion (kg oil eq).

The impacts are directly associated with the selectivity and specific productivity of fermentation. From the selectivity standpoint, a 20% increase results in reductions ranging from 1.5% to 5% in the analyzed categories, notably ODP with 4.8% and FD with 4.1%. However, negative variations in selectivity generate more pronounced positive variations in the analyzed categories, particularly ODP with 19.8% and GWP with 9.5%. This behavior is attributed to the increased demand for substrates in the process, requiring larger quantities to achieve the same amounts of SA. This increase leads to a higher demand for electricity compared to the base scenario due to the increased reaction volume.

Regarding productivity, variations tend to be slightly more proportional. A 20% increase in productivity results in impact reductions ranging from 1% to 7.1%, while a decrease generates increments between 1.6% and 11.9% in impact. This observation occurs because, with the increase in specific productivity, the reaction medium requires a smaller quantity of cells to produce the same amount of SA. This reduction results in a decreased reaction medium and, consequently, a lower demand for electrical energy.

The sensitivity analysis, involving a 20% increase and decrease in the process's energy demand, revealed noteworthy insights. Unlike the trends observed in the two previous analyses, variations in the energy demand led to proportional changes in environmental impacts. The impacts showed fluctuations ranging from 0.9% for ODP to a maximum of 16% for HTP, with a global average variation of about 5%. Notably, in terms of GWP, reducing the process's energy demand could result in up to a 4.5% decrease in carbon emissions. Regarding the distribution in energy demand, it is observed that the main share is related to the fermentation stage due to reactor agitation and the need for steam in reactor cleaning. These results underscore the pivotal role of the fermentation stage in the overall energy demand.

The benefits of fermentation improvement highlight the significant impact this stage has on the entire process. What happens in fermentation defines both upstream and downstream processes, as changes interfere with the demands of both stages. Positive results should be complemented by an economic analysis, establishing a relationship

between the costs associated with developing these improvements and the economic and environmental benefits.

3.3. Comparison of the Studied Scenarios

The comparison between the 1G process of producing SA from sugarcane juice with the other scenarios studied is presented in Table 1. The highest scores in each impact category are highlighted in gray color for illustrative purposes. Figure 6 presents a comparison of the highest impact value among the four SA production scenarios analyzed.

Table 1. LCA results of the succinic acid production scenarios. The highest scores in each impact category are highlighted in gray for illustrative purposes.

Categories	Units	1st Scenario	2nd Scenario	3rd Scenario	4th Scenario
AP	kg SO ₂ eq	2.35 × 10 ⁻²	1.04 × 10 ⁻²	1.26 × 10 ⁻²	12.9 × 10 ⁻²
EP	kg P eq	2.53 × 10 ⁻⁴	7.24 × 10 ⁻⁴	5.98 × 10 ⁻⁴	25.4 × 10 ⁻⁴
GWP	kg CO ₂ eq	1.95 × 10 ⁻¹	19.4 × 10 ⁻¹	13.4 × 10 ⁻¹	45.3 × 10 ⁻¹
ODP	kg CFC-11 eq	4.54 × 10 ⁻⁸	12.2 × 10 ⁻⁸	16.0 × 10 ⁻⁸	15.6 × 10 ⁻⁸
POP	kg NMVOC	11.8 × 10 ⁻³	6.10 × 10 ⁻³	5.33 × 10 ⁻³	46.4 × 10 ⁻³
HTP	kg 1,4-DB eq	6.43 × 10 ⁻²	3.67 × 10 ⁻²	6.04 × 10 ⁻²	46.0 × 10 ⁻²
AEP	kg 1,4-DB eq	2.05 × 10 ⁻²	4.70 × 10 ⁻²	2.16 × 10 ⁻¹	7.26 × 10 ⁻¹
TEP	kg 1,4-DB eq	8.98 × 10 ⁻⁴	233 × 10 ⁻⁴	240 × 10 ⁻⁴	3.53 × 10 ⁻⁴
MD	kg Fe eq	4.27 × 10 ⁻²	3.26 × 10 ⁻²	35.7 × 10 ⁻²	330 × 10 ⁻²
FD	kg oil eq	1.64 × 10 ⁻¹	4.48 × 10 ⁻¹	5.82 × 10 ⁻¹	21.1 × 10 ⁻¹

AP—acidification potential; EP—eutrophication potential; GWP—global warming potential; ODP—ozone depletion potential; POP—photochemical oxidation potential; HTP—human toxicity potential; AEP—aquatic ecotoxicity potential; TEP—terrestrial ecotoxicity; MD—metal depletion; FD—fossil depletion.

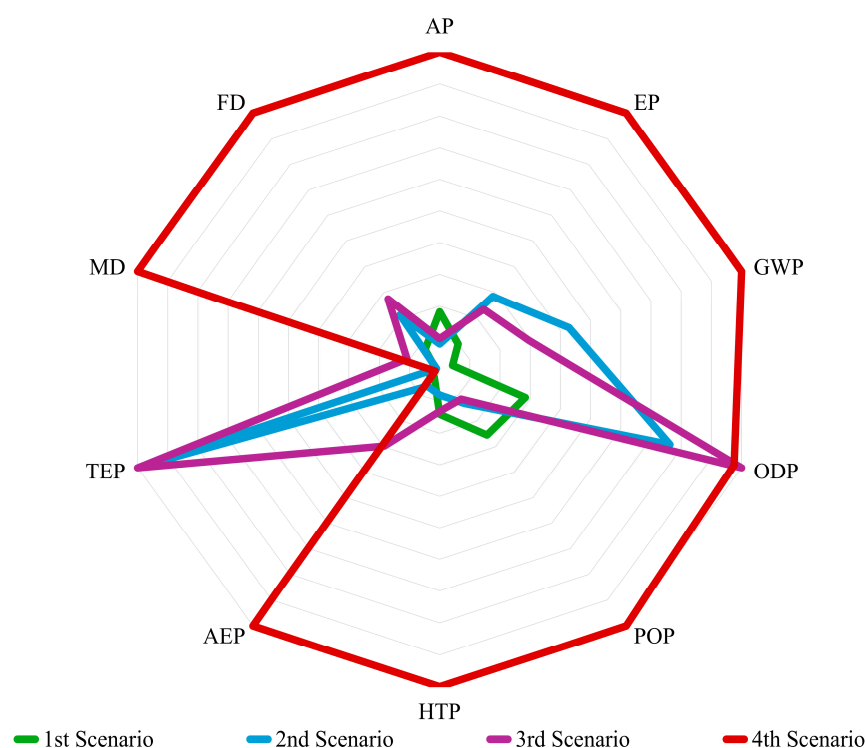


Figure 6. Comparison of the environmental performance of different routes of succinic acid production. AP—acidification potential; EP—eutrophication potential; GWP—global warming potential; ODP—ozone depletion potential; POP—photochemical oxidation potential; HTP—human toxicity potential; AEP—aquatic ecotoxicity potential; TEP—terrestrial ecotoxicity; MD—metal depletion; FD—fossil depletion.

In general, the impacts were strongly linked to the purification stage due to the high level of purity required—99.5% [12]. However, the upstream process, which considers the agricultural stage, stood out in the sugarcane and sorghum routes. The 1G process from sugarcane presented lower environmental impacts in most of the categories when compared to the other three scenarios. The contributions referring to sugarcane cultivation were substantially lower than for sorghum, which was related to the plant's adaptability to Brazilian soil, as well as its higher ethanol yield per hectare, as evidenced by Miranda and Fonseca [40]. The 1G process with sorghum, used by Myriant (2nd Scenario), has a higher contribution from the agricultural step when compared to the sugarcane process, since the planting of sorghum requires larger quantities of fertilizers such as glyphosate, with sorghum requiring 1 kg per ton compared to just 0.2 g for sugarcane, as observed in the inventories analyzed. This triggered impacts in almost all categories analyzed. The high use of ammonia also contributes to greater ecotoxicity impacts, with the amount used in the sorghum process being 27 times higher than in the sugarcane process. The higher demand for energy of the 2nd Scenario, which is around 2.67 kWh per kg of SA produced compared to 1.19 kWh for the 1st Scenario, adds up to impacts in most categories, even though the Brazilian energy matrix is predominantly renewable. In this sense, the search for alternatives for the sorghum used in the process can reduce the impacts generated during the cultivation stage.

The chemical route (4th Scenario) showed the highest impacts in most of the impact categories due to the use of maleic anhydride derived from petroleum and metal catalysts whose production is associated with impacts in all categories analyzed. The use of maleic anhydride has associated emissions of up to 2.4 kg of CO₂ emitted for every 1 kg of salt produced. This amount is higher than all the global emissions from the other scenarios, which highlights the damage caused by the use of oil derivatives. According to Kumar et al. [41], the process is not sustainable in the long term due to the price and availability of maleic anhydride, which is likely to worsen in the coming years considering international initiatives to reduce oil use. This makes the replacement of the process for alternatives with renewable inputs even more necessary and imminent.

The 2G process presented low impact indexes in most categories, showing itself to be an excellent alternative from the environmental point of view. The typical assumption of the null environmental burden for residual feedstocks, such as apple pomace, leads to lower results. In this case, the robust purification process is the largest contributor to the overall performance due to the large use of inorganic salts and sulfuric acid, exceeding the rates of the 1st Scenario, which has an associated agricultural stage. Sulfuric acid makes a strong contribution in the ecotoxicity categories, where its impacts represent up to 71.3% of the overall impacts of the process. In relation to salts, the contributions reach between 20 and 40% in all the categories analyzed. The development of the downstream steps, aiming at reducing the complexity and the use of substances, can facilitate the implementation of the process and help reduce the environmental impacts.

4. Discussion

The results underscore the importance of a comprehensive assessment of biomass selection, as it directly impacts environmental factors. The use of substances such as fertilizers and pesticides significantly contribute to overall environmental impacts for both sugarcane and sorghum. This recognition highlights the intricate relationship between the choice of biomass, fermentation conditions, and subsequent purification processes, necessitating a comprehensive optimization strategy.

In the context of Brazil, the utilization of sugarcane juice as a carbon source for fermentation emerges as a favorable option due to its lower environmental impacts and abundant availability. The simplified processing, along with reduced pre- and post-treatment steps, positions sugarcane as a superior choice compared to alternative crops [42]. Using the sugarcane-based process, the environmental impacts of SA would decrease between 70% and 99% compared to the petrochemical route. The presence of sugarcane companies and

Brazilian expertise further reinforces its status as the optimal choice, promoting environmental sustainability and supporting the growth of sugarcane-based products and biorefineries.

Among the scenarios evaluated, the stage with the strongest contributions to environmental impacts is downstream. Purification processes remain intricate due to the high level of purity necessary for marketing SA. In biotechnological processes, various steps are required to remove cells, water, and fermentation by-products and to carry out crystallization. A study conducted by Dessie [43] surveyed the literature on different innovative techniques for purifying SA produced via biotechnological routes. Membrane filtration techniques, which allow for purification directly from the fermentation broth itself with high selectivity and efficiency, are among the most promising alternatives [41,44,45]. Adsorption processes such as ion-exchange chromatography and adsorption on activated carbon have also yielded positive results for the separation of SA [46,47]. Crystallization [48] and liquid-liquid extraction [49] are other techniques that have been employed. The implementation of these technologies into production processes can lead to reduced impacts. The advantages are associated with the simplified operation, resulting in fewer processes required to reach the desired level of purity.

Enhancements in the fermentation process, such as increased conversion and greater selectivity for SA, can improve the economic and environmental performance of the process. Studies documented in the literature have demonstrated positive outcomes in terms of higher conversions of sugars into SA. For instance, while the yield of the 1st scenario reached 0.53 g of SA per g of substrate, whereas some works in the literature report 0.8 g/g of yield using sugarcane molasses and *A. succinogenes* [50] and up to 1.27 g/g with *E. coli* and glucose [51].

In addition to the environmental benefits of sugar cane SA compared to other pathways, the production costs of this scenario are also interesting. In the 1st scenario, using sugarcane, the minimum selling price is estimated at USD 2.89/kg (value from Furlan et al. [25] updated for 2023), a value comparable to the market price (ranging from USD 1.96/kg to USD 2.94/kg [16,31]). Biotransformation pathways, exemplified by the 2nd scenario, exhibit an average cost ranging from USD 2.86/kg to USD 2.94/kg. Meanwhile, chemical routes, represented by the 4th scenario, demonstrate an average cost between USD 1.96/kg and USD 2.00/kg [31]. Unfortunately, the 3rd scenario results from a conceptual study that lacks an economic analysis, which precludes the estimation of associated costs. However, 2G processes face challenges in terms of economic feasibility due to several bottlenecks, as highlighted by Magalhães [52], including a low substrate conversion from waste-derived materials, difficulties in waste storage, significant effluent volumes, transport constraints, and costs associated with biomass pre-treatment. These complicated economic considerations underline the complexity associated with the feasibility of 2G processes. Therefore, the 1st scenario also demonstrates economic potential, achieving a cost comparable to the international market price. However, it is crucial to note that this process is open to improvement and that ongoing development may contribute to a reduction in costs.

Future research should focus on creating new LCA inventories, building upon the most promising outcomes in the literature related to SA production and purification. These studies need to transition from lab-scale to industrial-scale modeling, incorporating data from successful literature results to provide insights into the environmental feasibility of large-scale renewable SA production. The envisioned LCAs should consider factors such as locale-specific raw material selection, microorganism optimization, and the configuration of a less complex purification process. By visualizing and analyzing the environmental results comprehensively, these studies have the potential to guide more sustainable and economically viable biotechnological pathways for large-scale SA production.

5. Conclusions

The use of sugar cane as a raw material for the production of SA in Brazil has shown significant environmental benefits, reducing the environmental impact when compared

to other production alternatives. The agricultural phase has significant environmental impacts due to the use of pesticides and fertilizers, but these are relatively modest when compared to other crops such as sorghum. The fermentation stage places high demands on energy, either electricity or heat. However, the impacts are mitigated by the energy from burning the sugarcane bagasse. The purification stage is robust due to the strict purity requirements for commercialization, which require substantial equipment, inputs, and energy demand. A careful selection of carbon sources and the development of efficient microbial platforms can minimize the formation of by-products and the presence of impurities after fermentation, thus reducing the need for separation steps. This holistic approach demonstrates the significant potential of SA production from sugarcane juice as an ecological and sustainable alternative.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/su16031234/s1>, Table S1: Inventory of the industrial stage of SA production from sugarcane; Table S2: Inventory of sugarcane juice production; Table S3: Distribution of inputs for each stage of the industrial process for producing succinic acid from sugar cane; Table S4: Inventory of the industrial step of SA production from sorghum; Table S5: Inventory of the agricultural stage of sorghum production in Brazil; Table S6: Inventory of the industrial stage of second-generation SA production in Brazil; Table S7: Inventory of SA production from the chemical route; Table S8: Inventory of maleic anhydride production; Figure S1: Flowchart of succinic acid production from first-generation sugarcane; first-generation sorghum; second-generation apple pomace and chemical route maleic anhydride.

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