

## Article

# Techno-Economic and Life Cycle Assessment of a Small-Scale Integrated Biorefinery for Butyric-Acid Production in Chile

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**Abstract:** This study evaluates the techno-economic and environmental feasibility of a small-scale biorefinery in Chile's La Araucanía Region, which utilizes wheat straw as feedstock to produce butyric acid using *Clostridium tyrobutyricum*. Two scenarios were considered; the standalone wheat straw biorefinery and its integration with the anaerobic digestion of pig manure for biogas production, coupled with a cogeneration system, using the xylo-oligosaccharides and lignin obtained in the pretreatment. The simulations were carried out using Aspen Plus, while the Aspen Process Economic Analyzer was used to perform the economic evaluation. The simulation results were validated with experimental data from the literature. An economic assessment was performed considering the different processes involved. A cradle-to-gate life-cycle analysis (LCA) was also applied to evaluate the different environmental impacts. Both studied scenarios were economically feasible, with the highest butyric acid production cost being USD 2.97/kg<sub>butyricacid</sub>; however, this value is still higher compared to corn-based biorefineries. Annexed biogas production increased the costs and was less economically attractive. Nonetheless, the integrations with biogas production had lower environmental impacts, except in the photochemical oxidant formation category, which was higher because of the combustion gases obtained by the cogeneration system. A lower carbon footprint (23.5 kg CO<sub>2</sub>-eq. per ton of wheat straw) was obtained for the scenario including biogas production.

**Keywords:** butyric acid; biorefinery; process simulation; LCA



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## 1. Introduction

The effects of climate change and the demand for chemicals and fuels produced from fossil resources have triggered the need to find substitutes obtained from biomass through sustainable biorefineries. Usually, the proposed biorefineries use a single feedstock with high processing capacities to achieve the maximum economy of scale. However, many reports have shown that the main bottlenecks are associated with high capital costs (CAPEX) and operating costs (OPEX), and very often lack biomass supply due to the amounts that must be available for the operation. To overcome those issues, biorefineries at a small scale have been proposed as a solution to deal with those challenges. When located in rural areas, they can promote the local economy and generate jobs directly and indirectly [1,2]. Moreover, the possibility of integration, i.e.: the processing of more than one residual material as feedstock to increase the economic or environmental feasibility of the operation, increases at small scales. The performances of the biorefineries can be evaluated by process modeling and simulation using software-based tools, as this is a useful methodology to ascertain process feasibility at both the pilot and industrial scales [2].

Butyric acid is a four-carbon fatty acid, and its commercial production is dominated by chemical synthesis from fossil resources. The advances in the fields of biotechnology and fermentation technologies have resulted in renewed attention to butyric acid production

from low-cost residues and renewable biomass [3,4]. Butyric acid is regarded as a prospective chemical building block for a variety of chemical compounds, and its derivatives have numerous potential applications in the chemical, textile, plastic, food, beverage, dairy, and pharmaceutical industries [5–7]. It is also considered a promising specialty chemical, as it can be converted to butanol [8]. In addition, the high amount of lignocellulose biomass as a lowly valuable agricultural commodity and the obligation of treatment of biowastes have been creating a favorable business climate for butyric acid fermentation [9].

The aim of this study was to assess the viability of utilizing two abundant resources in the Araucanía Region, Chile—wheat straw and swine manure—for the production of butyric acid. Wheat straw can be transformed into fermentable sugars and then to butyric acid by *Clostridium tyrobutyricum*. On the other hand, swine manure presents potential for biogas production via anaerobic digestion, offering a renewable energy source to enhance the overall energy efficiency of the biorefinery [10]. This study evaluates two distinct scenarios: Scenario 1, which involves the transformation of wheat straw into fermentation products without biogas generation, and Scenario 2, which integrates biogas production into the heat and power generation process. For both scenarios, a techno-economic analysis (TEA) and an environmental impact evaluation by life cycle assessment (LCA) were carried out to identify the most sustainable option.

## 2. Materials and Methods

### 2.1. Feed Stock Availability and Location

The main lignocellulosic residues in Chile are related to the production of wheat, corn, potatoes, and beets [11,12]. About 80–90% of wheat straw is burned [13], leading to detrimental consequences for climate change and human health [14,15], while less than 20% is used for energy generation [16]. Moreover, its generation is concentrated in the region of La Araucanía, where there are approximately 250,000 ha dedicated to this crop [11], with a productivity reaching up to 5.6 t ha<sup>-1</sup>. In the same region, there are several livestock farms with an estimated daily production of 160 m<sup>3</sup> of swine manure [17,18]. A study by Hetz et al. (2006) unveiled that a staggering 94% of producers resorted to incinerating all or a portion of their wheat straw, while a smaller group of producers (40%) found alternative uses for wheat straw, such as animal feed, bedding, and wind protection. An even smaller proportion (33%) adopted the practice of incorporating straw into the soil to enhance its quality [19]. Table 1 shows the composition of wheat straw [2,20,21].

**Table 1.** Wheat straw composition (on a dry weight basis).

Compounds	Cellulose	Hemicellulose	Lignin	Extractives	Ashes	Proteins
% w/w	36.8	25.9	17.1	14.5	4.7	1.0

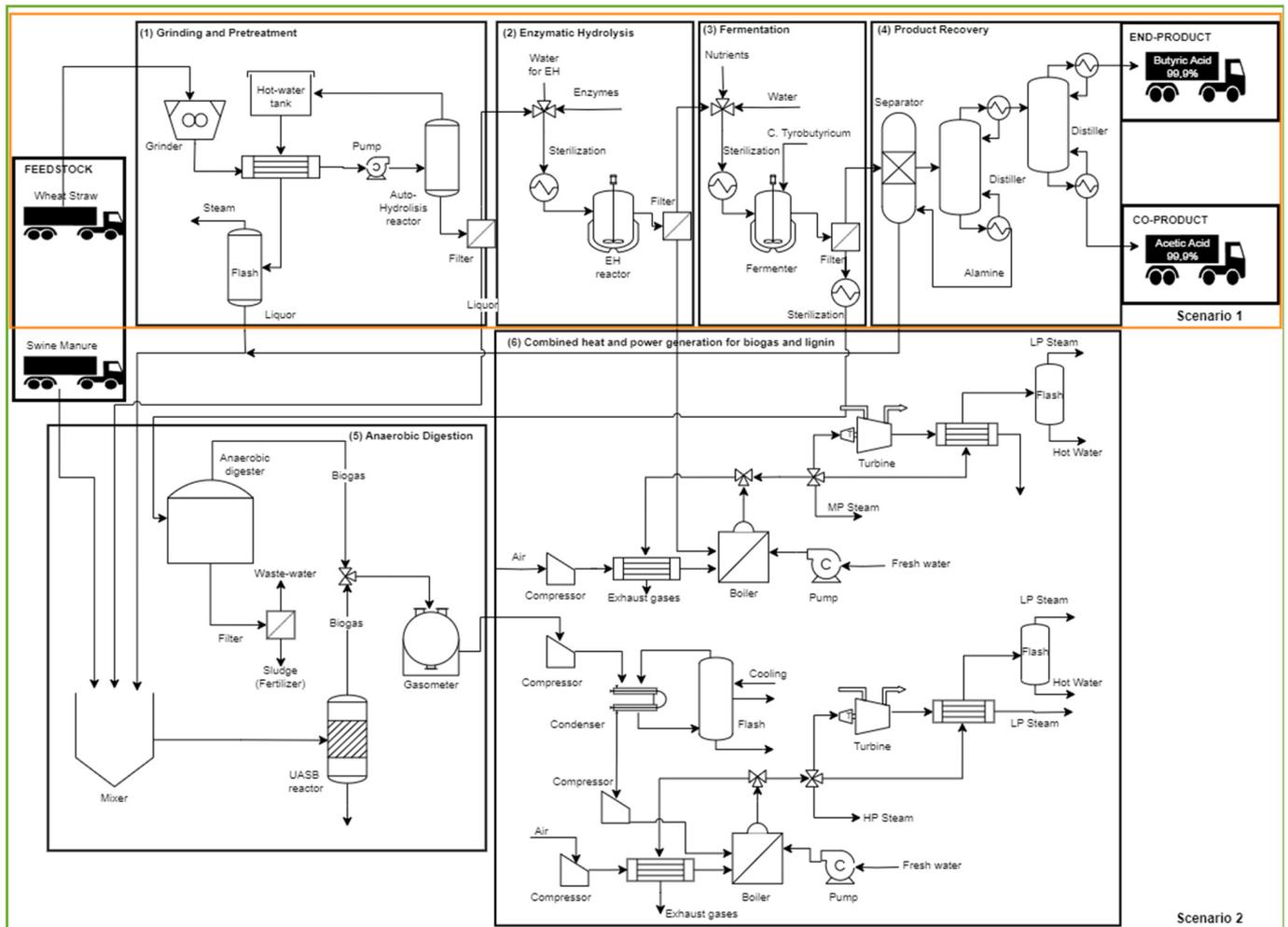
According to the availability of residues, a plant located at Victoria City in the region of La Araucanía could potentially have access to 32,000 tons per year of wheat straw [11] and 51,200 m<sup>3</sup> per year of swine manure [17].

### 2.2. Process Overview and Design

Wheat straw is pretreated by autohydrolysis, yielding a cellulose-rich pulp and a liquor containing oligomeric sugar, rich in xylo-oligosaccharides, which can be used for biogas production. The cellulosic pulp is enzymatically hydrolyzed, and the glucose syrup that is produced is fermented by an engineered strain of *Clostridium tyrobutyricum* to produce butyric acid. Residual cellulolignin solids are used for energy generation in a combined heat and power plant (CHP), and the spent broth and biomass from the fermentation can be combined with swine manure in an anaerobic bioreactor to produce biogas.

Figure 1 shows a flowsheet of the proposed integrated biorefinery process. The process is divided into six sections: (1) grinding and pre-treatment, (2) enzymatic hydrolysis,

(3) fermentation, (4) product recovery, (5) wastewater treatment and anaerobic digestion, and (6) combined heat and power generation from biogas and lignin.



**Figure 1.** Process flow diagram used to model butyric acid production, identifying the boundaries of the wheat straw standalone scenario (in orange) and the integrated biorefinery (in green).

Two scenarios were evaluated: the transformation of wheat straw into fermentation products without biogas generation (Scenario 1) and the integration of biogas in the heat and power generation process (Scenario 2). The lignin and xylo-oligosaccharides generated in Scenario 1 were considered waste streams rather than co-products.

### 2.2.1. Grinding and Pre-Treatment

The lignocellulosic biomass was milled by a crusher into particle less than 6 mm in size to obtain a high contact surface and reduce cellulose crystallinity [18] and was then pretreated by autohydrolysis at 19 bar and 210 °C with a solids-to-steam ratio of 1:8 [19]. Table 2 shows the hydrolysis reactions and the conversions considered.

**Table 2.** Stoichiometric reactions and fractional conversions for each process area involved.

Reaction Type	Stoichiometry	Fractional Conversion
Autohydrolysis [22]	Cellulose + H <sub>2</sub> O → Glucose	0.11
	Cellulose → HMF + 2 H <sub>2</sub> O	0.01
	Xylan + H <sub>2</sub> O → Xylose	0.88
	Xylan → Furfural + 2 H <sub>2</sub> O	0.11
	Arabinan + H <sub>2</sub> O → Arabinose	1.00
	Galactan + H <sub>2</sub> O → Galactose	1.00
	Acetate → Acetic Acid	1.00
Enzymatic Hydrolysis [23]	Cellulose + H <sub>2</sub> O → Glucose	0.99
	Cellulose + 0.5 H <sub>2</sub> O → 0.5 Cellobiose	0.01
	Cellobiose + H <sub>2</sub> O → 2 Glucose	1.00
	Xylan + H <sub>2</sub> O → Xylose	0.86
Fermentation [5]	0.175 Glucose + 0.2 NH <sub>4</sub> <sup>+</sup> → Biomass + 0.05 CO <sub>2</sub> + 0.45 H <sub>2</sub> O	0.15
	Glucose → Butyric Acid + 2 CO <sub>2</sub> + 2 H <sub>2</sub>	0.7
	Glucose → 3 Acetic Acid	0.15
	0.21 Xylose + 0.2 NH <sub>4</sub> <sup>+</sup> → Biomass + 0.05 CO <sub>2</sub> + 0.45 H <sub>2</sub> O	0.15
	3 Xylose → 2.5 Butyric Acid + 5 CO <sub>2</sub> + 5 H <sub>2</sub>	0.7
	2 Xylose → 5 Acetic Acid	0.15

### 2.2.2. Enzymatic Hydrolysis (EH)

Enzymatic hydrolysis (EH) was performed at 50 °C using Cellic® CTec3 cellulase (Novozymes, Bagsvard, Denmark) at 10 mg/g cellulose and 20% of solids loading, according to the conditions reported by the National Renewable Energy Laboratory (NREL) [24]. The EH reactions and fractional conversions considered are summarized in Table 2. At the end of the hydrolysis, after approximately 72 h, the lignin-rich solids were recovered by filtration and conveyed to CHP, whereas the glucose-rich stream was sent to fermentation.

### 2.2.3. Fermentation

Before fermentation, corn steep liquor was added to the hydrolysate and the culture medium was sterilized at 121 °C. The fermentation was performed by the microorganism *Clostridium tyrobutyricum*, and the initial concentration of glucose, the main carbon and energy source, was 70 g/L. The fermentation was carried out at 37 °C with a pH controlled at 6.0, and the fermentation lasted 70 h [25]. In accordance with Baroi et al. [5], the key fermentation products were H<sub>2</sub>, CO<sub>2</sub>, butyric acid, and acetic acid. Fermentation reactions are summarized in Table 2.

### 2.2.4. Product Recovery

Several operations have been proposed for the extraction of butyric acid from the fermentation broth, among others: liquid–liquid extraction, extractive fermentation, electro-dialysis, pervaporation, and salting-out; however, the most studied and promising method was liquid–liquid extraction [26]. Kang et al. [27] patented a method using trialkylamine (alamine-336) to form an insoluble complex with the anions of organic acids in the broth. This complex remained in the solvent (organic phase) and was separated from the broth (aqueous phase) by a gravity settler at 35 °C [28]. The butyric acid (BA) in the organic phase was then separated from alamine-336 by reactive distillation. The distillate contained high BA concentration, while the solvent was recovered at bottom stream due to the high difference in their boiling points [27]. The partition coefficients were 3.3 for BA and 0.55 for AA, using alamine-336 as solvent at an alamine-336-to-BA molar ratio of 5 [28].

### 2.2.5. Wastewater Treatment and Anaerobic Digestion

Wastewater streams (such as condensed pretreatment stream, permeate stream from solid–liquid separations, and downstream organic residual streams) were recovered, and due to the low chemical oxygen demand (COD), a UASB anaerobic reactor was selected for

its treatment. This bioreactor operated at 36 °C, with a hydraulic retention time of 18 h. The wet biomass and swine manure, together with the spent broth from the fermentation, were treated in an stirred anaerobic bioreactor with a residence time of 40 days at a temperature of 36 °C. The stoichiometric reactions considered for modeling the AD were based on the model proposed by Angelidaki et al. [29].

#### 2.2.6. Combined Heat and Power Generation for Biogas and Lignin

The lignin-rich solids generated in the pretreatment were dried until reaching 5% moisture, then burned in a boiler at 1540 °C with 10% of excess O<sub>2</sub> to produce high-pressure (HP) steam (24 bar), medium-pressure (MP) steam (4.4 bar), hot water, and electricity from steam expansion in a turbine. Furthermore, the biogas from anaerobic digestion was burned in a boiler over 1700 °C, with 20% of excess O<sub>2</sub>. The exhaust gases were expanded in a turbine to generate electricity while the generated steam inside the boiler was sent to a system like the one used for biomass to produce MP steam and hot water.

#### 2.3. Process Simulation

Mass and energy balances were obtained through simulation using Aspen Plus v12.1 (Aspen Technology Inc., Bedford, MA, USA). The thermodynamic model used in the simulations was the non-random two liquids (NRTL) model, and the state equation of Hayden O'Connell was used to describe the vapor phase. The properties of lignocellulosic components and microorganisms (such as cellulose, hemicellulose, lignin, enzymes, and bacteria) were taken from the NREL report [30]. To estimate flows, 7680 h (320 working days) per year were considered.

The economic evaluation of the biorefinery was carried out by estimating the capital cost, operating costs, and profitability for an expected scenario of 60% co-financing. Equipment purchase costs were estimated using the Aspen Process Economic Analyzer software v12.1 (Aspen Technology Inc., Bedford, MA, USA). In addition, cost correlations were used for the reactor, with and without stirring, and manufactured using stainless steel 304 or 316 [31].

The estimation of the capital cost considered direct and indirect costs; these were calculated according to the literature [32]. Direct costs were calculated based on the costs of the equipment and its installation, plus the cost of the buildings, site preparation, and piping, which were estimated based on a percentage of the auxiliary equipment (ISBL). Indirect costs were calculated based on a percentage of total direct costs, and maintenance cost was estimated as 6% of the total investment cost [24]. The economic evaluation was conducted for a 20-year operation in Chile, with a minimum return rate of 4%, an inflation of 2.6% per year, and an income tax of 27% (2023) [33].

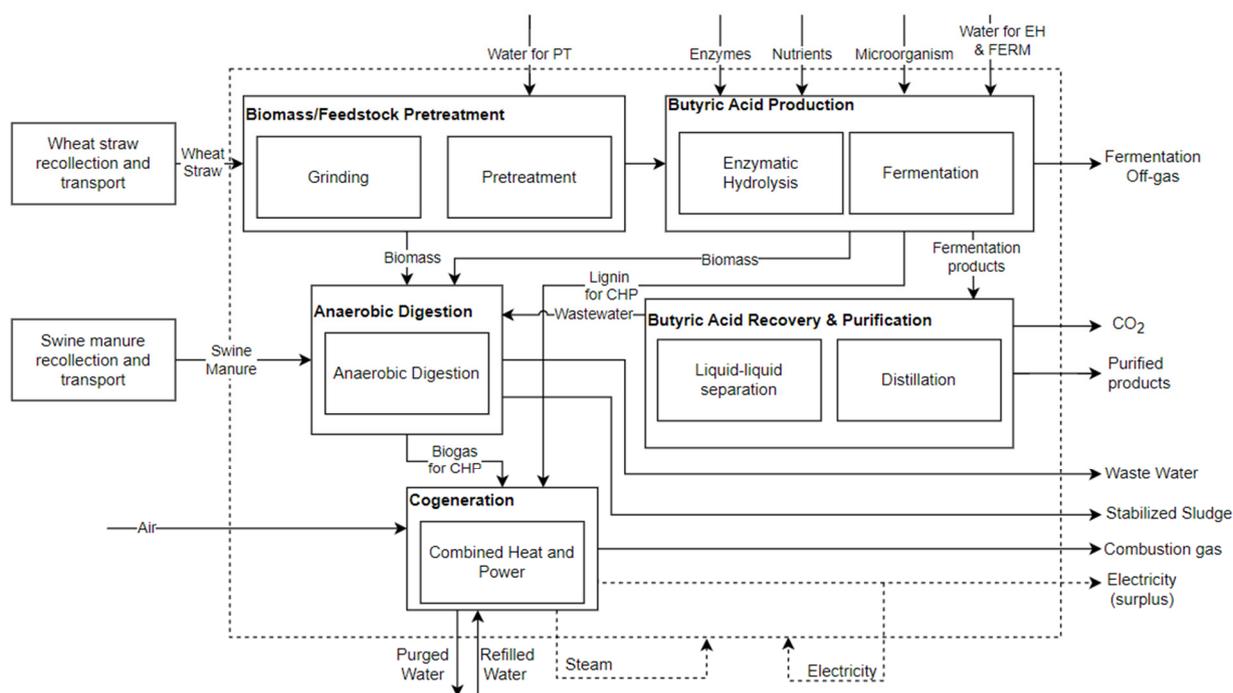
#### 2.4. Life-Cycle Assessment (LCA)

To comprehensively assess the environmental implications of the biorefinery's entire life cycle, an LCA was conducted for both scenarios, enabling a sustainability comparison between wheat straw cultivation and the production and disposal of bioproducts.

For the LCA, the functional unit was 1 kg of lignocellulosic feedstock, which was assessed from cradle to gate using SimaPro software v9.5 and the ReCiPe Midpoint (H) method.

The scope and boundaries of this LCA were wheat straw cultivation, harvesting, transportation, and preprocessing, along with the environmental impacts of swine manure infrastructure and transportation, if applicable. Additionally, it evaluated the environmental performance of biorefinery bioconversion, separation, and purification processes, including the transportation and application of supplies. Finally, it encompassed the environmental impacts associated with waste management.

Figure 2 shows the system boundaries considered for the LCA, as well as the inputs and outputs for the process. For comparative purposes, both wheat straw and butyric acid (100% allocation) were considered as functional units, and the inventory flows which were considered can be found in the Supplementary Materials.



**Figure 2.** Process system boundaries for life cycle assessment of integrated biorefineries (cradle to gate). Lines represent: (---) system boundary; (→) mass streams; (- ->) energy streams.

### 3. Results and Discussion

#### 3.1. Process Simulation

The simulation results demonstrated a feasible production of 2295 tons/year of butyric acid and 20 tons/year of acetic acid, both at 99.9% purity. Calculations were made on a glucose and xylose yield basis of 0.372 and 0.0988 g/g for butyric and acetic acid, respectively.

Table 3 shows the electrical and thermal energy balances for each biorefinery area. The pretreatment area consumed most of the thermal energy due to the high-pressure steam required for hydrothermolysis. The cogeneration area demanded most of the electrical energy, especially for the pumps and compressors designed to supply medium- and high-pressure steam to the rest of the plant. Nevertheless, the results from the net balance indicate that the process was self-sufficient in terms of heat and electricity due to the cogeneration processes, generating a surplus that could be sold to the grid (scenario 2). The HP steam cogeneration process generated 3.93 MW of heat, which was directly utilized in the hydrothermolysis process. Simultaneously, it produced 397 kW of electricity. The medium-MP steam cogeneration process produced 8.83 MW of heat, which was employed for heating purposes within the plant, while also generating 108 kW of electricity.

**Table 3.** Energy balances for butyric acid biorefinery.

Area	Electric Balance (kW)	Heat Balance (MW)
(1) Grinding and Pretreatment	44.8	3.93
(2) Enzymatic Hydrolysis	1.1	0.41
(3) Fermentation	0.9	1.91
(4) Product Recovery	0.2	1.33
(5) Anaerobic Digestion	14.2	0.42
(6) Combined Heat and Power	−169.0	−12.73
Net Balance (Scenario 1)	47.0	7.56
Net Balance (Scenario 2)	−107.8	−4.75

### 3.2. Economic Assessment

#### 3.2.1. Operating Expenditures (OPEX)

Scenario 2 has the potential to inject electricity into the grid, which would generate an income. In contrast, scenario 1 requires energy from the electrical grid and heating from natural gas combustion, which increased operating costs. Table 4 shows the expenses for raw materials, supplies, and services, as well as the revenues for product sales for each scenario. Cellulose enzymes represent the most significant operational expense, accounting for 14% and 13% of the OPEX for scenarios 1 and 2, respectively. However, enzyme costs are primarily determined by the supplier, and enzyme production is beyond the scope of this study. Therefore, a reduction in production costs was achieved by increasing the butyric acid yield through key process analysis, as discussed at the end of this section.

The total revenues for scenarios 1 and 2 were USD 6.76 and 7.35 million/year, respectively. This difference is mainly due to the sale of stabilized sludge for agricultural purposes.

Unlike scenario 2, which has an anaerobic digestion system to treat the effluents, the effluents of the scenario 1 must have their organic load reduced. Consequently, an additional cost for the operation of a wastewater preliminary treatment plant was estimated from the cost functions proposed by Ozgun et al. [34], resulting in a cost of USD 1.22 USD m<sup>3</sup> of effluent for a plant capacity of 1062 m<sup>3</sup>/day. A similar cost of USD 1.28/m<sup>3</sup> was estimated by Abbasi et al. [35] for a wastewater treatment plant with a capacity of 5000 m<sup>3</sup>/day.

**Table 4.** Expenses, revenues flows, and prices for butyric acid production.

Input/Product Name	Flows <sup>1</sup>		Price	Price Ref.	
	Scenario 1	Scenario 2			
Expenses on Raw Material, Supplies, and Utilities	Water	44.591 ton/h	62.240 ton/h	0.73 USD/ton	[36]
	Electricity	47.024 kW	-	29.60 USD/GJ	[37]
	Natural Gas <sup>2</sup>	7.560 MW	-	5.35 USD/GJ	[38]
	Alamine-336	1.286 kg/h	1.286 kg/h	8.49 USD/kg	[39]
	Swine Manure	-	5.244 ton/h	29.88 USD/ton	[40]
	Corn Liquor	88.180 kg/h	88.180 kg/h	52.10 USD/ton	[2]
	CTec3 Enzyme	12.130 kg/h	12.130 kg/h	10.14 USD/kg	[41]
	Wheat Straw	4.167 ton/h	4.167 ton/h	35.00 USD/ton	[2]
Product Revenues	Electricity	-	107.754 kW	29.60 USD/GJ	[37]
	Butyric Acid	0.299 ton/h	0.299 ton/h	2888.59 USD/ton	[42]
	Acetic Acid	0.027 ton/h	0.027 ton/h	617.00 USD/ton	[8]
	Stabilized Sludge	-	1.703 ton/h	39.00 USD/ton	[43]

<sup>1</sup> Flow estimation considered 7680 h per year. <sup>2</sup> Considering 1000 BTU per m<sup>3</sup> of natural gas and 85% conversion efficiency.

Table 5 summarizes the production costs of butyric acid, excluding co-products. The calculated production cost was lower than that reported by Baroi et al. [44], which was estimated to be USD 3.31 per kg of butyric acid at 99% purity.

The main differences between the two studies are the dependence on external energy sources and the product extraction method used (reverse electro-enhanced dialysis). In addition to the lower production cost, the proposed scenario also has the economic advantage of producing acetic acid, stabilized sludge as fertilizer, and electrical energy, which are not considered in the calculation of the unit production cost.

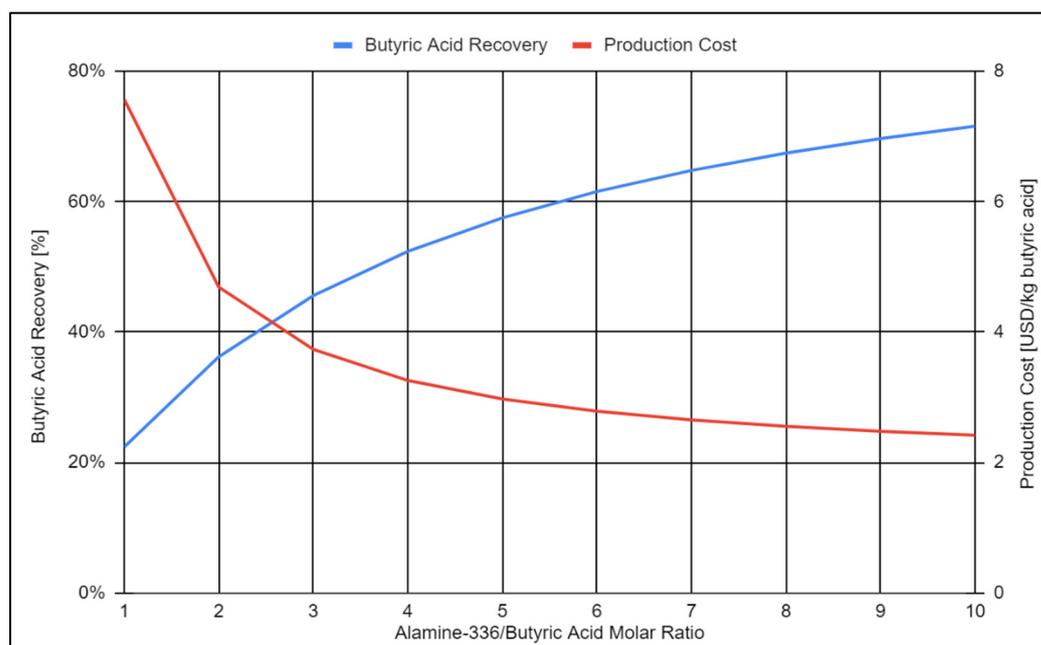
To diminish production costs, an increase in the butyric acid yield from 0.39 to 0.43 g/g in *C. tyrobutyricum* becomes feasible by diminishing the catabolite repression on xylose initial consumption due to high glucose concentrations [45]. In that study, a production cost of USD 1.65/kg was estimated for 2000 tons/year of butyric acid from a corn biorefinery, 60% and 80% lower compared to scenarios 1 and 2, respectively. Sensitivity analyses were conducted to identify the key process that significantly impacted production costs, revealing that the amount of butyric acid recovered through extraction and reactive distillation using alamine-336 played a crucial role. The heat available for the integrated biorefinery limited

the molar ratio of alamine-336 to butyric acid to a maximum of 10. Figure 3 shows the results of the sensitivity analysis, suggesting that the production cost can be reduced by about 20% by doubling the amount of alamine-366 used in the liquid–liquid extraction process. Additional experimental data will be required in order to elucidate the impact of increasing the extractant concentration upon the composition of the mixture, particularly the simultaneous extraction of butyric and acetic acids. Its impact upon the purity of the mixture after the solvent is recovered by reactive distillation should also be assessed.

**Table 5.** Cost estimation for butyric acid production.

Cost	Scenario 1	Scenario 2	Unit
Raw Materials and Utilities	4.00	3.73	USD million/year
Maintenance	1.25	1.89	USD million/year
Labor, Management, and Administrative	0.55	0.74	USD million/year
Capital depreciation <sup>1</sup>	0.27	0.46	USD million/year
Total	6.08	6.83	USD million/year
Butyric acid production cost (excluding co-products)	2.65	2.97	USD/kg

<sup>1</sup> Calculated using the straight-line method.



**Figure 3.** Sensitivity analysis, production cost, and butyric acid recovery based on the alamine-336-to-butyric-acid molar ratio for Scenario 2.

Subtracting operating expenses (OPEX) from product revenues resulted in operating profits of USD 0.951 and 0.986 million/year for scenarios 1 and 2, respectively. These results indicate that annualized cash flows for the operating income were better for the biorefinery scenarios integrated with wheat straw and swine manure, mainly due to their heat and power self-sufficiency.

3.2.2. Capital Expenditures (CAPEX)

In this study, the total capital cost for scenario 2 was estimated considering the following operations: (1) grinding and pre-treatment, (2) enzymatic hydrolysis, (3) fermentation,

(4) product recovery, (5) wastewater treatment and anaerobic digestion, and (6) combined heat and power generation from biogas and lignin. Scenario 1 excludes areas (5) and (6), but includes a wastewater pretreatment plant, which was estimated using the cost functions proposed by Ozgun et al. [34]. All the equipment costs and economic assessment datasheets are presented in the Supplementary Materials. Table 6 presents a summary of the CAPEX investment costs.

**Table 6.** Investment cost summary.

Item	Scenario 1 (USD Million)	Scenario 2 (USD Million)
Equipment Purchase Cost	5.40	9.16
Inside Battery Limits Plant Cost	9.26	11.33
Additional Direct Cost	1.62	1.98
Installed Equipment Cost	10.31	16.06
Total Direct Cost (TDC)	11.93	18.04
Total Indirect Cost (TIC)	8.95	13.53
Total Investment Cost (TIC + TDC)	20.88	31.57

The main difference between the proposed scenarios in terms of equipment costs relied mainly on the centrifugal compressors required for the biogas use in the cogeneration area (USD 2.19 million).

Baroi et al. [44] estimated a capital cost of USD 53.68 million for a 10000 ton/year butyric acid plant from wheat straw. Because the cost of the equipment exceeded 50% of the capital cost, a gross estimation applying the six-tenth rule [46] (a scale factor of 0.6) revealed that the cost of the same plant for 2295 ton/year of butyric acid was USD 22.20 million. Regarding this value, the biorefinery integrated with wheat straw and swine manure was 42% more expensive, while the standalone wheat straw biorefinery was 6% cheaper. Note that this estimate does not consider any of the obtained co-products, unlike the reference study, which had no additional products.

### 3.2.3. Total Costs and Economic Evaluation

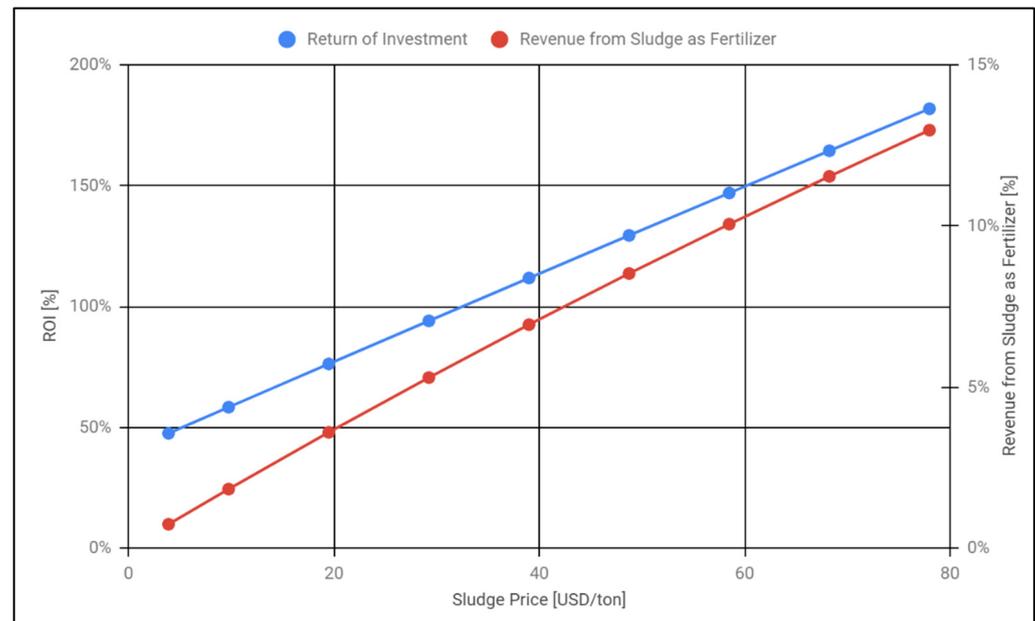
After calculating the CAPEX and OPEX, the projects were evaluated using different metrics, including payback period, net present value, and internal rate of return. The results are shown in Table 7.

**Table 7.** Summary of economic profitability measures for each project.

	Scenario 1	Scenario 2	Unit
Total Capital Investment	20.88	31.57	USD million
Credit Annualized Value (60% external financing)	0.99	1.49	USD million/year
Operating Expenditures (OPEX)	5.80	6.37	USD million/year
Product Revenues	6.76	7.35	USD million/year
Payback Period	8.61	10.60	years
IRR (After Taxes)	16.40	12.80	%
Net Present Value (NPV)	24.69	24.92	USD million
Return of Investment (ROI)	176	112	%

Although the net present value from the integrated biorefinery scenario was slightly higher than the standalone wheat straw biorefinery scenario (0.9%), the total capital investment was 51.2% higher. Thus, the payback period, internal rate of return, and return of investment were considerably lower for the biorefinery scenario integrated with wheat straw and swine manure.

Although scenario 2 had the lowest profitability, the variation in the additional co-products could be analyzed. Figure 4 shows how the return on investment (ROI) varied with the price of stabilized sludge. The price ranged from 10% to 200% of the reference price (USD 39 per ton). The results suggest that doubling the sludge price would increase the ROI of scenario 2 by 63% (from 112% to 182%), making it more profitable than scenario 1 (176%). This price also increased the revenue share from stabilized sludge by 87%, which led to a 54% increase in the net present value (NPV) (from USD 24.92 to 38.47 million).



**Figure 4.** Variation in wheat-straw- and swine-manure-integrated biorefinery ROI based on the price of stabilized sludge as fertilizer.

To assess the feasibility of using dry stabilized sludge as a fertilizer, it is necessary to perform an elemental analysis to determine its nutrient content. This can be compared to the nutrient content of commercial fertilizers to assess its potential value. For example, from January to March 2023, fertilizers fortified with urea, phosphate, and potassium had an average market value of USD 491/ton [47]. If the dry stabilized sludge had a similar nutrient content, it could potentially be used as a valuable fertilizer alternative.

These scenarios serve as initial benchmarks for assessing the feasibility of the process. Exploring additional valorization pathways for the xylo-oligosaccharides and lignin-rich solids obtained from the biorefinery process could significantly enhance overall profitability. For instance, employing ion-exchange chromatography and nanofiltration could facilitate the extraction and purification of xylo-oligosaccharides, suitable for applications as prebiotics or functional food ingredients [2]. Alternatively, modifying the structures of lignin-rich solids to improve their reactivity and bonding properties could enable their utilization in the production of high-value products, such as adhesives or bio-based composites [48].

Furthermore, refining the methods used for investment calculation could involve adopting a more comprehensive life cycle costing approach. This approach promotes a shift from an exclusive focus on the “best value for money” to a more holistic assessment that considers the entirety of an asset’s value throughout its life cycle [49].

### 3.3. Life Cycle Impact Assessment (LCIA)

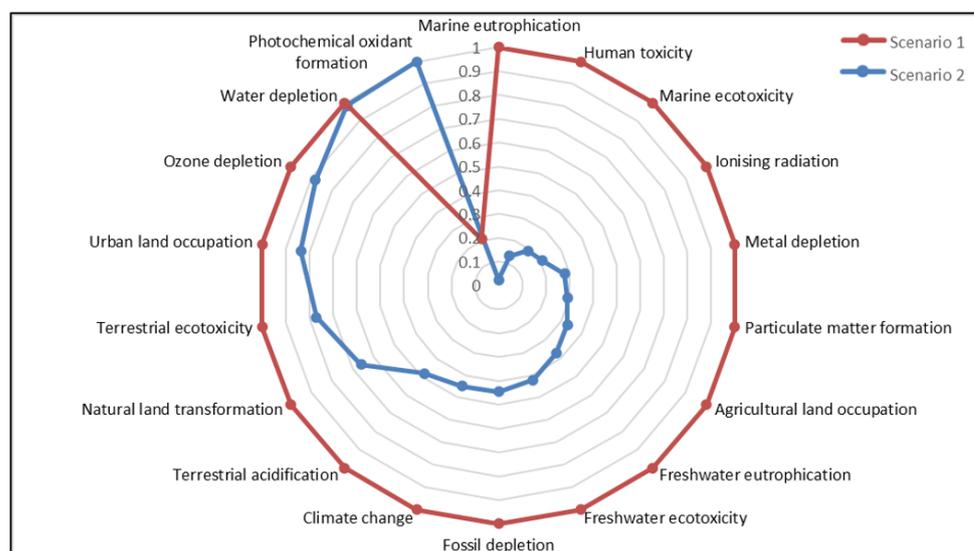
The mass and energy balances for the life-cycle inventory, as well as the considered inventory flows, are presented in detail in the Supplementary Materials for both scenarios.

Regarding climate change (CC), the integrated biorefinery had an impact of 0.327 kg CO<sub>2</sub>-eq./kg butyric acid, while the standalone wheat straw biorefinery had a

total CC impact of 0.727 kg CO<sub>2</sub>-eq./kg butyric acid, more than double the impact of scenario 2. Câmara-Salim et al. [50] conducted a life-cycle assessment for the previously mentioned butyric acid from wheat straw biorefinery [44], achieving 6.89 kg CO<sub>2</sub>-eq./kg butyric acid. This was mainly due to the production method, which implies the intensive use of electricity for the extraction method and the utilization of sulfuric acid, sodium, and potassium hydroxides, accounting for the major contributions to the climate change impact (at least 45%).

A life cycle assessment of isobutene and xylo-oligosaccharides for a wheat-straw- and swine-manure-integrated biorefinery reported a climate change impact on 0.76 kg CO<sub>2</sub>-eq./kg wheat straw [2], which is also higher than the 0.0235 kg CO<sub>2</sub>-eq./kg wheat straw calculated in this study. This is mainly due to two factors: (1) the emission gases were nearly 5 times higher than the amount of wheat straw processed, while in this study, that proportion was halved to 2.6; and (2) a major proportion of the CO<sub>2</sub> was not considered biogenic, which implies a greater climate change impact [41].

Figure 5 shows the different impacts, normalized by their maximum values, to facilitate comparison across multiple impact categories and provide a proportional comparative view for each impact category.



**Figure 5.** Comparison of ReCiPe midpoint (H) method impacts divided by the maximum value between both scenarios.

The integrated biorefinery had lower impacts for all impact categories except photochemical oxidant formation, which was five times higher for the integrated biorefinery (Table 8). This is mainly due to the emission of flue gas from the cogeneration system, mainly differentiating due to the presence of nitrogen oxides, which had an impact 10 times higher for the second scenario than the disposal of lignin for incineration did for the second scenario (see Supplementary Material). Integrated biorefinery scenario 2 consistently demonstrated lower environmental impacts, thus suggesting a more sustainable approach.

Regarding CC, cellulase enzyme production and transport contributed with 0.166 kg CO<sub>2</sub>-eq./kg butyric acid, accounting for 51% of the climate change impact of scenario 2. For further process optimization, producing fungal cellulases on-site is a promising strategy for reducing the environmental impact and cost of the integrated biorefinery, as they can be produced from low-cost feedstocks and locally (on-site), which eliminates the need to transport them from long distances.

However, it is crucial to acknowledge the need for uncertainty analysis in this LCA study. Uncertainty analysis quantifies the variability of data and its influence on the results, affecting both inventory data and impact assessment indicators; it stems from both errors and inherent fluctuations in the data [51]. While the impact of data variability on how

LCA results are used for decision making could provide valuable insight, it has not been explored in this study.

To fully encompass the triple-bottom-line framework of sustainability (environmental, economic, and social), the United Nations Environment Programme (UNEP) advocates for incorporating the perspectives of workers, consumers, local communities, society, and value chain actors through a social life cycle assessment (S-LCA) to understand the impact on human capital, human well-being, cultural heritage, and social behavior [49,52].

**Table 8.** Summary of environmental impacts calculated by the ReCiPe midpoint (H) method.

Impact Category	Unit	Per kg of Butyric Acid Produced		Per kg of Wheat Straw Processed	
		Scenario 1	Scenario 2	Scenario 1	Scenario 2
Human toxicity	kg 1.4-DB eq	$3.194 \times 10^{-1}$	$4.192 \times 10^{-2}$	$2.29 \times 10^{-2}$	$3.01 \times 10^{-3}$
Ionizing radiation	kBq U <sub>235</sub> eq	$1.187 \times 10^{-2}$	$2.500 \times 10^{-3}$	$8.52 \times 10^{-4}$	$1.79 \times 10^{-4}$
Particulate matter formation	kg PM <sub>10</sub> eq	$3.228 \times 10^{-3}$	$9.368 \times 10^{-4}$	$2.32 \times 10^{-4}$	$6.72 \times 10^{-5}$
Freshwater eutrophication	kg P eq	$3.777 \times 10^{-4}$	$1.405 \times 10^{-4}$	$2.71 \times 10^{-5}$	$1.01 \times 10^{-5}$
Fossil depletion	kg oil eq	$2.350 \times 10^{-1}$	$1.049 \times 10^{-1}$	$1.69 \times 10^{-2}$	$7.52 \times 10^{-3}$
Terrestrial acidification	kg SO <sub>2</sub> eq	$7.638 \times 10^{-3}$	$3.679 \times 10^{-3}$	$5.48 \times 10^{-4}$	$2.64 \times 10^{-4}$
Terrestrial ecotoxicity	kg 1.4-DB eq	$9.151 \times 10^{-5}$	$7.069 \times 10^{-5}$	$6.56 \times 10^{-6}$	$5.07 \times 10^{-6}$
Ozone depletion	kg CFC-11 eq	$8.490 \times 10^{-8}$	$7.492 \times 10^{-8}$	$6.09 \times 10^{-9}$	$5.37 \times 10^{-9}$
Photochemical oxidant formation	kg NMVOC	$3.863 \times 10^{-3}$	$1.874 \times 10^{-2}$	$2.77 \times 10^{-4}$	$1.34 \times 10^{-3}$
Water depletion	m <sup>3</sup>	$2.116 \times 10^{-1}$	$2.084 \times 10^{-1}$	$1.52 \times 10^{-2}$	$1.50 \times 10^{-2}$
Urban land occupation	m <sup>2</sup> a	$1.326 \times 10^{-2}$	$1.111 \times 10^{-2}$	$9.51 \times 10^{-4}$	$7.97 \times 10^{-4}$
Natural land transformation	m <sup>2</sup>	$9.909 \times 10^{-5}$	$6.569 \times 10^{-5}$	$7.11 \times 10^{-6}$	$4.71 \times 10^{-6}$
Climate change	kg CO <sub>2</sub> eq	$7.270 \times 10^{-1}$	$3.272 \times 10^{-1}$	$5.21 \times 10^{-2}$	$2.35 \times 10^{-2}$
Freshwater ecotoxicity	kg 1.4-DB eq	$9.260 \times 10^{-3}$	$3.899 \times 10^{-3}$	$6.64 \times 10^{-4}$	$2.80 \times 10^{-4}$
Agricultural land occupation	m <sup>2</sup> a	$3.978 \times 10^{-3}$	$1.317 \times 10^{-3}$	$2.85 \times 10^{-4}$	$9.45 \times 10^{-5}$
Metal depletion	kg Fe eq	$3.188 \times 10^{-2}$	$8.925 \times 10^{-3}$	$2.29 \times 10^{-3}$	$6.40 \times 10^{-4}$
Marine ecotoxicity	kg 1.4-DB eq	$8.702 \times 10^{-3}$	$1.648 \times 10^{-3}$	$6.24 \times 10^{-4}$	$1.18 \times 10^{-4}$
Marine eutrophication	kg N eq	$3.190 \times 10^{-3}$	$7.502 \times 10^{-5}$	$2.29 \times 10^{-4}$	$5.38 \times 10^{-6}$

#### 4. Conclusions and Future Works

Although both scenarios show positive profitability under the considered economic evaluation parameters, economic indicators clearly indicate that the most profitable option is scenario 1, which uses only wheat straw as a raw material. However, a more precise characterization of the content of stabilized sludge for its potential use as a fertilizer could transform scenario 2, which integrates the use of pig manure for producing biogas, into the most profitable one.

The butyric and acetic acid recovery can be improved by increasing the amount of alamine-336 used for the liquid–liquid separation; it would be an improvement for the wheat straw biorefinery, but still, the production cost would not be competitive compared to corn or corn husk biorefineries.

The use of solvent extraction followed by reactive distillation results in a significant reduction in environmental impact compared to other processes that produce butyric acid or biorefineries based on wheat straw. In addition, the energy self-sufficiency of an integrated biorefinery (Scenario 2) provides a lower environmental impact in most of the evaluated categories compared to a wheat-straw-only biorefinery (Scenario 1).

In conclusion, the proposed integrated biorefinery has the potential to be more profitable and sustainable over time by integrating different feedstocks to achieve energy self-sufficiency and extraction processes with low environmental impact.

Future works will focus on the optimization of downstream and valorization processes, as well as uncertainty quantification of TEA and LCA. Furthermore, a better understanding of the impact on this decision could be achieved by incorporating life cycle costing (LCC) and social LCA (S-LCA) tools.

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