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Article

Exergy-Based Improvements of Sustainable Aviation Fuels: Comparing Biorefinery Pathways

Pablo Silva Ortiz [1,*], Silvio de Oliveira, Jr. [2], Adriano Pinto Mariano [3], Agnes Jocher [1] and John Posada [4,*]

[1] School of Engineering and Design, Technical University of Munich (TUM), 85748 Garching, Germany; agnes.jocher@tum.de
[2] Polytechnic School, University of São Paulo (USP), São Paulo 05508-270, Brazil; soj@usp.br
[3] Faculdade de Engenharia Quimica, Universidade Estadual de Campinas (UNICAMP), Campinas 13083-852, Brazil; adpm@unicamp.br
[4] Department of Biotechnology, Faculty of Applied Sciences, Delft University of Technology (TUDELFT), 2629 HZ Delft, The Netherlands
* Correspondence: pablo.silva@tum.de (P.S.O.); j.a.posadaduque@tudelft.nl (J.P.)

Abstract: The aeronautical sector faces challenges in meeting its net-zero ambition by 2050. To achieve this target, much effort has been devoted to exploring sustainable aviation fuels (SAF). Accordingly, we evaluated the technical performance of potential SAF production in an integrated first- and second-generation sugarcane biorefinery focusing on Brazil. The CO_2 equivalent and the renewability exergy indexes were used to assess environmental performance and impact throughout the supply chain. In addition, exergy efficiency (η_B) and average unitary exergy costs (AUEC) were used as complementary metrics to carry out a multi-criteria approach to determine the overall performance of the biorefinery pathways. The production capacity assumed for this analysis covers 10% of the fuel demand in 2020 at the international Brazilian airports of São Paulo and Rio de Janeiro, leading to a base capacity of 210 kt jet fuel/y. The process design includes sugarcane bagasse and straw as the feedstock of the biochemical processes, including diverse pre-treatment methods to convert lignocellulosic resources to biojet fuel, and lignin upgrade alternatives (cogeneration, fast pyrolysis, and gasification Fischer-Tropsch). The environmental analysis for all scenarios shows a GHG reduction potential due to a decrease of up to 30% in the CO_2 equivalent exergy base emissions compared to fossil-based jet fuel.

Keywords: exergy and environmental assessment; biojet fuel production; biorefinery performance measurement

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1. Introduction

The aviation industry accounted for 2% of the total global anthropogenic carbon dioxide (CO_2) emissions (approximately 859 million metric tons) in 2017, and long-term growth in the air transport sector is expected in the coming decades [1]. Therefore, the International Air Transport Association (IATA) recognizes the need to address the global challenge of climate change, primarily on Greenhouse Gas emissions, and has adopted a net-zero target by 2050 [2]. Moreover, the International Civil Aviation Organization (ICAO) agreed on the adoption of a global market-based scheme to limit international aviation carbon dioxide equivalent (CO_{2e}) emissions based on the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA). CORSIA has been framed to allow offsetting through the implementation of credits or using CORSIA Eligible Fuels (CEFs), such that international aviation achieves neutral carbon growth as of 2020. CEFs include so-called sustainable aviation fuels (SAFs) as well as lower-carbon aviation fuels (LCAFs). For commercial utilization, SAFs must comply with the American Society for Testing and Materials (ASTM) International standards to be considered a drop-in substitute for petroleum-based aviation fuel [3]. For that, biomass conversion pathways (i.e., ethanol/alcohol-to-jet—ATJ, hydroprocessed esters and fatty acids—HEFA, Fischer-Tropsch synthesis—FT, aqueous phase reforming—APR, direct sugar to hydrocarbon—DSHC, and hydrotreated depolymerized cellulosic jet—HDCJ) have been developed. Figure 1 shows promising pathways for biojet fuel production based on the conversion systems. For instance, the application of these pathways is a function of feedstock, typically recognized between lipid-based (such as camelina oil, jatropha, algae) and carbohydrate-based (such as sugarcane and lignocellulosic biomass) feedstocks. In addition, conversion processes for lipid-based feedstocks include mainly hydroprocessing technologies. In contrast, carbohydrate-based feedstocks are typically converted via biochemical (into sugars) or thermochemical pathways (into bio-oils) based on gasification or pyrolysis processes. Hence, several types of synthesis (fermentative or catalytic) could be applied to upgrade sugars, alcohols, and syngas into biojet fuel [4].

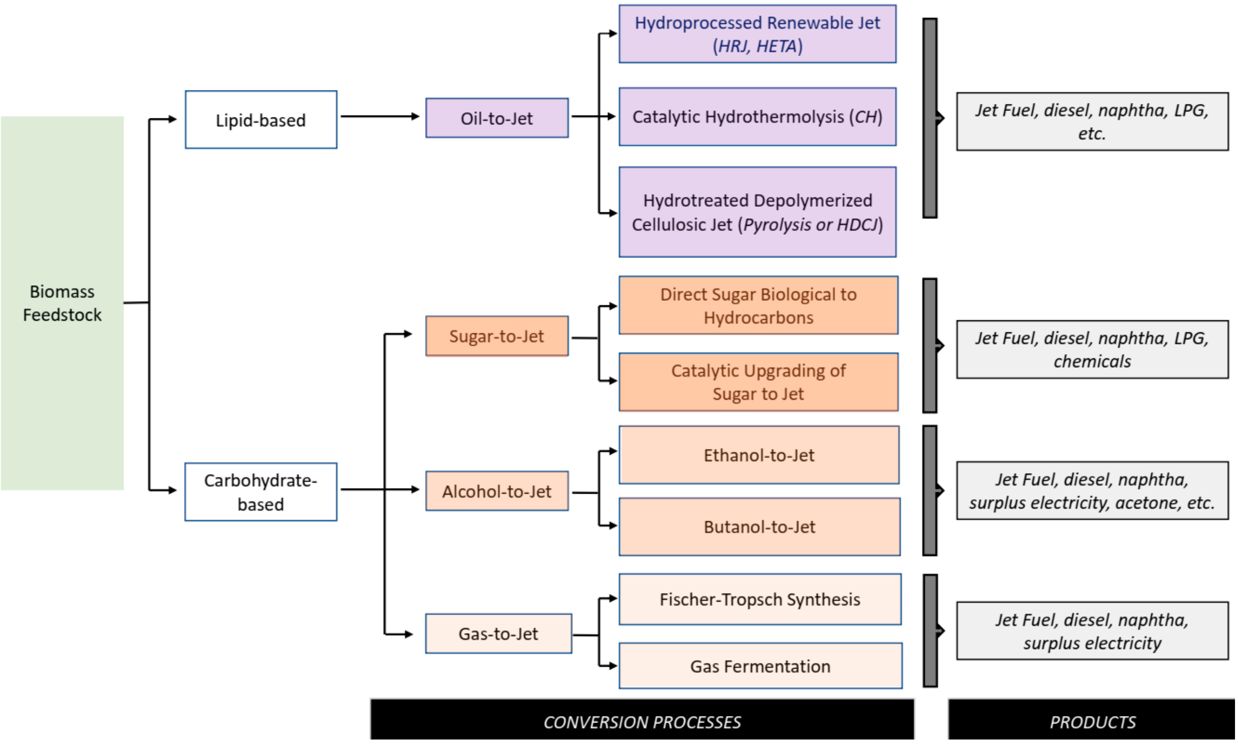


Figure 1. Overview of biojet fuel conversion routes. Classification based on feedstock, biomass conversion technology, and final product (adapted from [4]).

These production pathways have already been assessed in the literature for their economic and environmental performance in the context of various supply chains [5–7]. For instance, de Jong et al. [5] performed a supply scenario of non-food renewable jet fuel (RJF) in the European Union (EU) vision 2030 based on biomass availability, conversion technologies, regulatory conditions, and the biomass demand analysis from other sectors (i.e., power, transport, heat, and chemicals). Model scenarios show that non-food RJF supply could reach 3.8–6.1 million t/year (equal to 165–261 PJ/y) by 2030. Santos et al. [6] present a techno-economic analysis (TEA) and an environmental assessment (LCA) of the whole production chain (i.e., biomass production, sugar extraction, biomass pretreatment, sugars fermentation, and products recovery and purification) of a sugarcane-based biorefinery focused on biojet fuel production. The authors also compared multiple options for biomass pretreatment and biojet fuel production routes from sugars and biomass. GHG emissions and non-renewable energy use (NREU) were mainly lower than 42.5 $kgCO_{2eq}/GJ$ and 700 MJ/GJ for all scenarios, respectively. Michailos [7] promoted the production of farnesane from bagasse, aiming at diversifying energy supplies and mitigating the environmental impacts of the aviation sector from the lignocellulosic sugars pathway to biojet fuel. The results show a mass yield of 0.121 $kg_{jet\ fuel}/kg_{dry\ bagasse}$ and an energy efficiency of 26.5%. Cradle-to-grave GHG emissions reductions compared to fossil jet fuel can be approximately 47%.

Gerber et al. [8] presented a methodology to integrate LCA in thermo-economic models for the optimal conceptual design of energy conversion systems. De Jong et al., 2017 [9] compared the well-to-wake (WtWa) GHG emission performance of multiple renewable jet fuel (RJF) conversion pathways and explored the impact of different co-product allocation methods. The results show that FT yields the highest GHG emission reduction compared to fossil jet fuel (86–104%) of the pathways in scope, followed by Hydrothermal Liquefaction (77–80%) and sugarcane- (71–75%) and corn stover-based ATJ (60–75%). Capaz et al. [10] performed an attributional life-cycle assessment for ten RJF pathways in Brazil, considering the environmental trade-offs between climate change and other impact categories. The scope includes sugarcane and soybean for first-generation (1G) pathways and residual materials (wood and sugarcane residues, beef tallow, and used cooking oil) for second-generation (2G) pathways. Three certified technologies were analyzed: HEFA, ATJ, and FT. Results show that 1G pathways significantly reduce GHG compared to fossil kerosene from 55% (soybean/HEFA) to 65% (sugarcane/ATJ). Mussatto et al. [11] summarize and discuss different SAF technologies, their potential to be upscaled, and their techno-economic perspectives, as well as the comprehensive impact of SAF on sustainability from an industry point of view, focusing on the production and use of aviation biofuels.

In addition, the assessment of performance variables to accelerate the SAF deployment at different regional scales has been explored. Bhatt et al. [12] evaluated the implications of key variables including type and quantity of feedstock availability, SAF production cost, GHG emissions, and fuel/infrastructure logistics on the deployment of SAF in Chicago, USA. These authors demonstrated that woody biomass-based Fischer-Tropsch technology has the lowest fuel production costs of all pathways assessed, reducing GHG emissions by 86% compared to conventional jet fuel. Rojas Michaga et al. [13] evaluated the technical, economic, and environmental performance of a Power-to-Liquid (PtL) route for SAF production in the UK context. This SAF production system involves a direct air capture unit, an off-shore wind farm, an alkaline electrolyzer, and a processing plant (reverse water gas shift coupled with an FT reactor). A WtWa life-cycle assessment shows that the global warming potential (GWP) equals 21.43 g_{CO2eq}/MJ_{SAF}, and is highly dependent on the upstream emissions of the off-shore wind electricity. The study concludes by estimating the required monetary value of SAF certificates for different scenarios under the UK SAF mandate guidelines. Sacchi et al. [14] showed a climate-neutral aviation fly strategy for Europe based on LCA and a time-dependent quantification of non-CO_2 climate impacts. This study demonstrates from a technological standpoint that using electricity-based synthetic jet fuels and compensating for climate impacts via direct air carbon capture and storage can enable climate-neutral aviation.

However, while previous case studies have mainly focused on economic and environmental performances to identify the most promising SAF pathways, a multi-criteria approach based on complementary methods, such as exergy analysis, environmental assessment-GHG emissions, and renewability exergy measurement, has not yet been reported. This work presents a multi-criteria analysis to assess an integrated first- and second-generation sugarcane biorefinery for biojet fuel production in Brazil using performance indicators, namely exergy efficiency (η_B), carbon dioxide equivalents (CO_{2EE}), average unitary exergy costs (AUEC), and the renewability exergy indicator (λ). As case studies, we examine biochemical processes to convert lignocellulosic resources to biojet fuel and lignin upgrade alternatives (cogeneration, fast pyrolysis, and gasification Fischer-Tropsch). Hence, a systematic comparison based on exergy and environmental analyses, renewable percentage, and exergy costs was used to determine the overall performance of the biorefinery pathways.

2. Materials and Methods

Twenty-four (24) biorefinery pathways were selected and assessed based on a pre-screening phase of eighty-one (81) configurations covering the conversion of (*i*). first-generation (1G) sugar (sucrose) and (*ii*). sugarcane bagasse for either production of second-generation (2G) sugar or direct conversion into jet fuel.

The multi-criteria approach includes mass, energy, and exergy balances of each biorefinery system based on theoretical and empirical correlations to determine the thermodynamic properties in the models. Then, exergy efficiencies, exergy losses, and the exergy use/export, as well as the environmental metric (i.e., specific CO_2 equivalent emissions) related to the conversion processes, were considered performance indicators, allowing a systematic comparison based on an exergy-based analysis of the pathways. Hence, the interconnection among exergy and environmental analyses, renewable percentage, and exergy costs was used to determine the overall performance of the biorefinery scenarios. Mass, energy, and exergy balances were modeled in spreadsheets based on parameters [6] from a Brazilian modern plant. For the 2G production from bagasse, the following pre-treatment methods were assessed: dilute acid (DA), dilute acid + alkaline treatment (DA-A), steam explosion (SE), steam explosion + alkaline treatment (SE-A), organosolv (O), wet oxidation (WO), liquid hot water (LHW), and liquid hot water + alkaline treatment (LHW-A) [6]. Then, the resulting streams underwent detoxification and enzymatic hydrolysis to produce fermentable sugar. For lignin, three possibilities were considered: cogeneration (cogen), jet fuel production via fast pyrolysis (FPJ), and biojet fuel production via gasification Fischer-Tropsch (GFT). Moreover, auxiliary steps were analyzed for each biorefinery scenario based on the process data from Santos et al. [6], i.e., wastewater treatment (WWT) and H_2 steam methane reforming (H_2SMR). Tables A1–A4 present the technical parameters of the milling process, ethanol upgrade to jet process considerations, and operation parameters adopted in lignin fast pyrolysis and syngas Fischer-Tropsch. Lastly, Table A5 reports the main KPIs for each biorefinery (81 configurations) analyzed in the pre-screening step. Figure 2 shows a simplified flow chart of the processing sections and system boundaries adopted in this study.

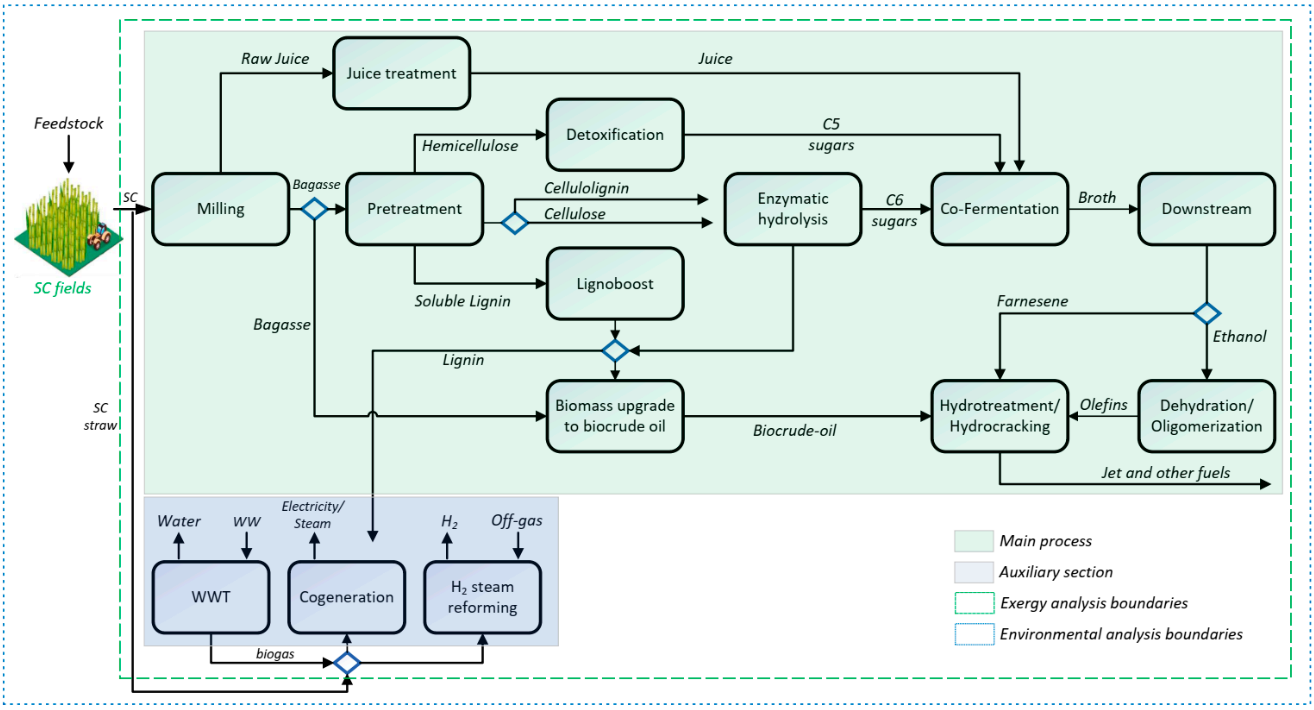


Figure 2. Processing sections and system boundaries for exergy and environmental analysis (adapted from Santos et al. [6]).

2.1. Production Technologies and Processing Conditions

A sugarcane field with a productivity of 12,000 t of sugarcane (SC) per day was selected as it represents the processing capacity of a typical sugarcane mill in São Paulo State (SP-Brazil) operating 200 days a year.

The biorefinery plant is divided into four areas: SC milling, bagasse pre-treatment, fermentation, upgrade (intermediate products to jet fuel/thermochemical upgrade of lignin and bagasse to jet fuel), and auxiliary sections (Figure 2). The cane is transported on a conveyor belt to the plant. In this first step, sugarcane is chopped and cleaned. The bagasse (lignocellulosic fraction) is divided from the sugarcane juice (liquid fraction). Then, the juice is processed into sugar and ethanol. Sugar is produced by evaporation, clarification, and crystallization stages. The remaining juice (molasses stream), a high concentration of fermentable sugars, is converted into ethanol by fermentation with yeast. Lastly, the ethanol obtained in the fermentation step is separated by distillation from hydrated ethanol (95 wt%) and then separated using molecular sieves to produce anhydrous ethanol (99.8 wt%).

More details about each unit system can be found elsewhere [6,15]; in these references, the process design and assessment of a sugarcane-based ethanol production system are presentedfocusing on traditional ethanol production (1G), mass-integrated (1G2G), and mass and heat-integrated systems.

2.2. Exergy Assessment

The exergy analysis method, which combines the First and Second Laws of Thermodynamics, was used to assess the efficiency of sugarcane-based biorefineries for jet fuel production. Exergy is a thermodynamic propriety that represents the maximum work that could be obtained through reversible processes from a system that interacts with the components of the environment until the equilibrium state (e.g., mechanical, thermal, and chemical) is attained [16]. Therefore, exergy analysis provides a rational metric for evaluating the quality and quantity of a given energy resource. Based on the prevailing environmental conditions, it denotes the maximum of this particular energy resource that can be converted into work [17].

Exergy Balance

The SC biorefinery scenarios are based on the steady-state mass, energy, and exergy balances for each control volume (see Equations (1)–(3)), referring to all inlet and exit matter streams, work, and heat transfers adopted in the assessment [18].

$$\sum_{inlet} \dot{m}_i = \sum_{outlet} \dot{m}_e \tag{1}$$

$$\sum_{inlet} \dot{m}_i h_i + \dot{Q}_{CV} = \sum_{outlet} \dot{m}_e h_e + \dot{W}_{CV} \tag{2}$$

$$\sum_{inlet} \dot{m}_i b_i + \dot{Q}_{CV_i}\left(1 - \frac{To}{T}\right) = \sum_{outlet} \dot{m}_e b_e + \dot{W}_{CV_e} + \dot{I} \tag{3}$$

where $\sum_{inlet} \dot{m}_i b_i$ denotes the exergy flow rate of the process inputs ($\dot{B}_{inputs}$), $\sum_{outlet} \dot{m}_e b_e$ the exergy flow rate of the process output ($\dot{B}_{products}$), and $\left(\dot{I}\right)$ the Irreversibility rate (exergy destroyed). In this study, both chemical (b_{CH}) and physical (b_{PH}) exergies are determined due to the physico-chemical processes included.

- *Exergy efficiency*: The exergy efficiency for the biorefinery pathways is determined by the ratio between the sum of exergy products and the sum of exergy resources as given in Equation (4) [19].

$$\eta_B = \frac{\sum \dot{B}_{products}}{\sum \dot{B}_{resources}} \tag{4}$$

- Irreversibility rate: The irreversibility rate was found by applying the exergy balance expression introduced in Equation (3). The specific exergy values [15] of the inputs considered were 5130 kJ/kg (SC), 16,725 kJ/kg (straw), and 9667 kJ/kg ($SC_{bagasse}$). Concerning the exergy of the products, the values adopted in the simulations of the analyzed plants were 17,479 kJ/kg (sugar) and 27,042 kJ/kg (bioethanol). The specific chemical exergies are usually close to their lower heating value (LHV) for fuels in reference conditions of temperature and pressure (T0 and P0). The relation between b_{CH} and LHV values for several fossils is mainly given in Szargut et al. [9], and for bio-based raw materials in Silva Ortiz et al. [8]. Table A6 shows the standard chemical exergy (b_{CH}) per resource adopted. The technological comparisons carried out in Section 3.2 are based on the exergy efficiency calculations of each scenario, where the exergy of the products and the inputs are established based on the relation between b_{CH} and LHV values.

2.3. Specific CO_2 Equivalent Emissions

The environmental analysis is comprised of calculations for GHG emissions in a cradle-to-gate approach plus the cogeneration unit boundaries concerning the exergy of the products. Energy allocation was employed to determine the specific GHG emissions of the production of jet fuel using the various biorefinery configurations. Individual environmental impact factors per type of process input are given in Table A6 (e.g., feedstocks and utilities). The impact assessment method selected was 'cane sugar production with ethanol by-product' (Brazilian case-Activity) [20], and the impact category 'Global Warming Potential (GWP 100 years)' was determined as an environmental performance indicator. Hence, the environmental factors combined with the exergy value of the products yield the CO_2 equivalent emissions in the exergy base (CO_{2EE}); see Equation (5) [21],

$$CO_{2\,EE} = \frac{\text{Global } CO_{2\,equivalent\ emissions}}{B_{\text{products}}} \tag{5}$$

2.4. Average Unitary Exergy Cost (AUEC)

AUEC represents the amount of exergy necessary to obtain one unit of product. AUEC is applied as a parameter to measure the cumulative irreversibility and exergy consumption, which occurs in the upstream processes to form a particular exergy stream [22]. Consequently, higher irreversibility translates into higher AUEC unit exergy costs. According to Equation (6), the average unit exergy cost c (kJ/kJ) of the biofuel production processes and the electricity can be established as the weighted average of the exergy costs of these products. More details about the unit exergy cost and exergy efficiency definitions applied to bioenergy systems are given in Silva Ortiz et al. [8].

$$AUEC_{process} = \frac{c_{biojet\ fuel} \times B_{biojet\ fuel} + c_{power} \times B_{power}}{B_{biojet\ fuel} + B_{power}} \tag{6}$$

2.5. Renewability Exergy Index

The exergo/environmental analysis concerning the renewability of biorefinery systems was conducted using the renewability exergy index (λ) [19]. The renewability index incorporates the exergy associated with the useful products ($B_{\text{products or co-products}}$) of a specified energy conversion process, the destroyed exergy ($B_{\text{destroyed}}$), the exergy associated with non-renewable inputs (B_{fossil}), the exergy required to dispose of wastes, and the exergy flows related to emissions, residues, and untreated wastes, as detailed in Equation (7). Thus, analyzing the renewability of energy conversion processes contributes to an assessment by using thermodynamic parameters [23].

$$\lambda = \frac{\sum B_{products\ or\ co-products}}{B_{fossil} + B_{destroyed} + B_{deactivation} + B_{disposal} + B_{emissions}} \tag{7}$$

The value of the λ index indicates (*i*). $0 \leq \lambda < 1$ for environmentally unfavorable processes; (*ii*). $\lambda = 1$ for internally and externally reversible processes with non-renewable inputs; (*iii*). $\lambda > 1$ for processes environmentally favorable; and (*iv*). $\lambda \to \infty$ for reversible processes with renewable inputs and no wastes generated. When the renewability exergy index is greater than 1, the $B_{products}$ can be used to "restore" the environment to the prevailing conditions before the process and still obtain a positive flow of exergy for another use. Note that λ is closely related to the control volume (CV) analyzed, due to the number of energy conversion processes involved. Hence, when the selected CV is expanded, the λ value decreases as a function of the irreversibility and the contribution of non-renewable (fossil) inputs to the process. It is essential to guarantee the compatibility of the CV when different systems are compared to prevent distortions during the evaluation. The interpretation of the renewability exergy index that focuses on bioethanol production routes is presented in Silva Ortiz et al. [21], which synthesizes the case studies related to biomass conversion via biochemical and thermochemical methods.

Usually, the application of exergy-based methods to measure the performance of biofuels refers to the evaluation of the exergy efficiency of biomass-to-biofuel conversion processes, including renewable and non-renewable resources. The sustainability and renewability of bioenergy processes involve many environmental and ecological aspects, such as emissions of greenhouse gases (e.g., the life-cycle assessment) or land-use changes. To quantify the degree of non-renewable resources in biofuel conversion processes, the exergy accounting should be performed over the entire bioenergy life cycle, from crop cultivation until the final biofuel is obtained in the conversion process [18]. Hence, the exergy concept became a key factor for various sustainability metrics for bioenergy systems [19] and biofuel production pathways [24,25].

3. Results and Discussion

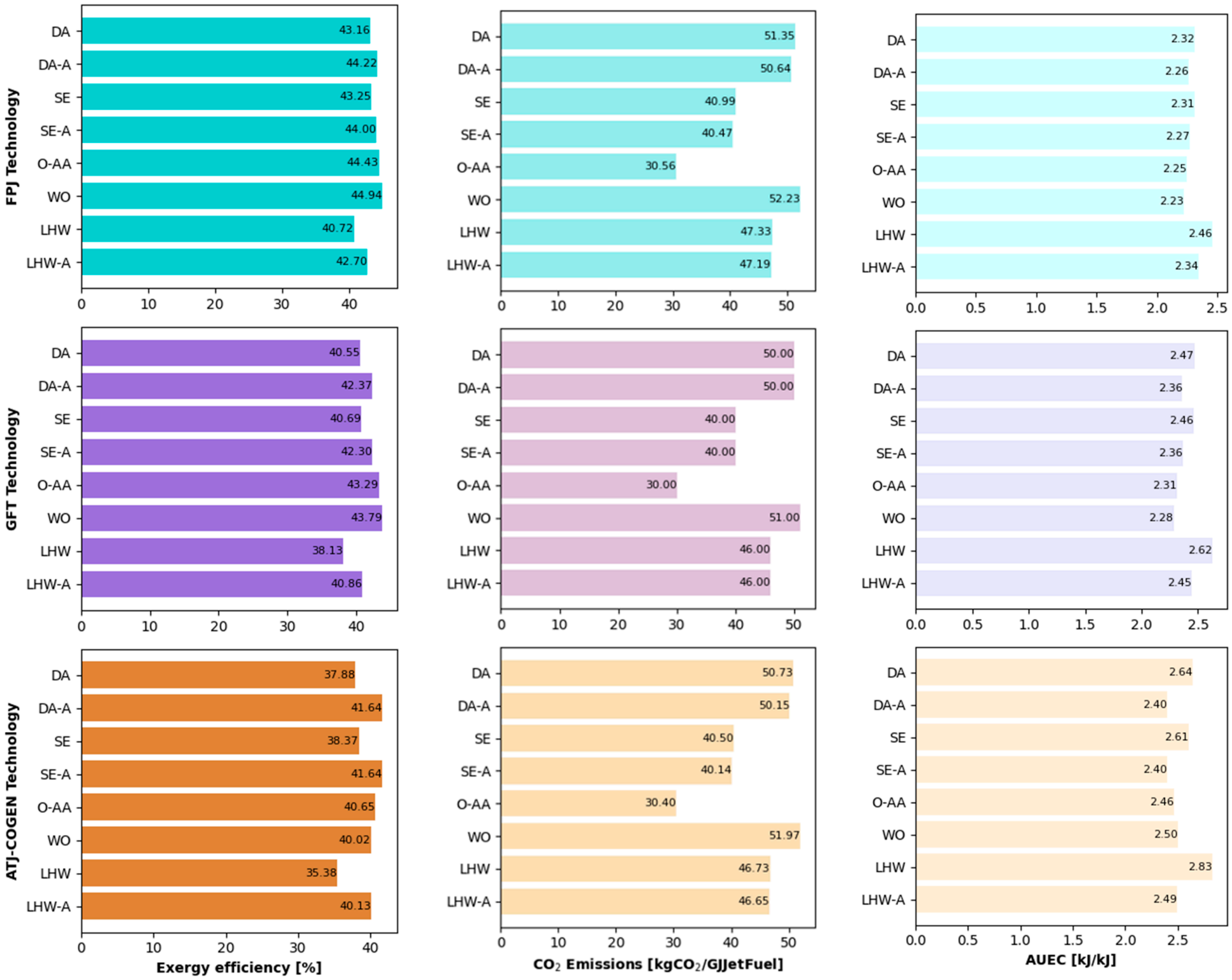
The processes were assessed based on the mass, energy, and exergy balances of the twenty-four (24) biorefinery pathways selected. These criteria were used to evaluate each scenario's performance according to technical, environmental, and economic exergy-based conditions.

3.1. Sugarcane Biorefineries Performance

The exergy performance for the twenty-four biorefinery scenarios is given in Figure 3. Overall, a better performance was obtained by combining the pre-treatment processes with the alkaline treatment (DA-A, SE-A, LHW-A) than by the lignocellulosic pre-treatments carried out alone (DA, SE, O, WO, and LHW). The main KPIs for each biorefinery analyzed in the pre-screening phase (81 configurations) are reported in the Appendix A section (Table A5).

In the bagasse pre-treatment methods, the wet oxidation (WO) process generated the highest exergy efficiency. The second-best pre-treatment option was organosolv (O-AA) for acetic acid recovery, which improves the biomass fiber conversion. Figure 3a shows the alternative uses for lignin (FPJ, GFT, and COGEN). The global exergy efficiency performed better for the scenarios that used fast pyrolysis (FPJ). Figure 3b depicts the specific CO_2 equivalent emissions in the exergy base for the sugarcane biorefinery pathways. All technologies should lead to at least a 30% decrease in environmental impacts compared to 85–95 kg CO_2 GJ^{-1} from conventional petroleum-based jet fuel [3].

Pathways employing dilute acid (DA), dilute acid + alkaline treatment (DA-A), and wet oxidation (WO) were ranked as having the highest emissions among the twenty-four scenarios. In contrast, steam explosion (SE), steam explosion + alkaline treatment (SE-A), and organosolv (O) remained consistently below the emission targets because of higher yields of jet fuel.



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

Figure 3. Performance indicators: (**a**) exergy efficiency; (**b**) specific CO_2 equivalent emissions; (**c**) AUEC.

Thus, by applying the CO_2 equivalent indicator and renewability exergy index, the exergy concept was used as an ecological metric to quantify the exergy losses and to determine the presence of emissions in the environment. In brief, the λ for the sugarcane biorefineries was environmentally unfavorable for all 24 scenarios, indicating that the exergy of the products cannot always be used to restore the environment to the conditions prior to operating the process, mainly due to the total irreversibility found in the jet fuel production and power generation processes.

Lastly, the exergy cost measures the cumulative irreversibility and exergy consumption (kJ/kJ). Thus, the AUEC was calculated for each biorefinery pathway focusing on jet fuel production (see Figure 3c). The lower exergy cost of the systems was obtained in the FPJ technology as an alternative to the lignin destination. Table 1 gives an overview of the primary KPIs for each renewable jet fuel scenario.

Table 1. Key performance indicators for the renewable jet fuel configurations [1].

Technology				*FPJ*				
Pre-treatment	**DA**	**DA-A**	**SE**	**SE-A**	**O-AA**	**WO**	**LHW**	**LHW-A**
Exergy efficiency (%)	43.16	44.22	43.25	44.00	44.43	44.94	40.72	42.70
Irreversibility rate (MW)	119	117	119	117	116	115	124	120
AUEC (kJ/kJ)	2.32	2.26	2.31	2.27	2.25	2.23	2.46	2.34
GHG emission $(\text{kgCO}_2/\text{GJ}_{\text{Jet Fuel}})$	51.35	50.64	40.99	40.47	30.56	52.23	47.33	47.19
λ	0.67	0.69	0.67	0.69	0.70	0.71	0.61	0.70
Technology				*GFT*				
Pre-treatment	**DA**	**DA-A**	**SE**	**SE-A**	**O-AA**	**WO**	**LHW**	**LHW-A**
Exergy efficiency (%)	40.55	42.37	40.69	42.30	43.29	43.79	38.13	40.86
Irreversibility rate (MW)	124	120	124	121	118	117	129	123
AUEC (kJ/kJ)	2.47	2.36	2.46	2.36	2.31	2.28	2.62	2.45
GHG emission $(\text{kgCO}_2/\text{GJ}_{\text{Jet Fuel}})$	50.73	50.15	40.50	40.14	30.40	51.97	46.73	46.65
λ	0.60	0.65	0.61	0.65	0.67	0.68	0.55	0.64
Technology				*ATF (COGEN)*				
Pre-treatment	**DA**	**DA-A**	**SE**	**SE-A**	**O-AA**	**WO**	**LHW**	**LHW-A**
Exergy efficiency (%)	37.88	41.64	38.37	41.64	40.65	40.02	35.38	40.13
Irreversibility rate (MW)	130	122	129	122	124	126	135	125
AUEC (kJ/kJ)	2.64	2.40	2.61	2.40	2.46	2.50	2.83	2.49
GHG emission $(\text{kgCO}_2/\text{GJ}_{\text{Jet Fuel}})$	50.00	50.00	40.00	40.00	30.00	51.00	46.00	46.00
λ	0.54	0.63	0.55	0.63	0.61	0.59	0.49	0.59

[1] They are determined based on the key performance indicators of Section 2.

Similarly, Figure 4 indicates that the λ index performed better for the biorefinery systems that use fast pyrolysis as a method to process lignin, confirming the relationship between the technological pathway renewability and the exergy performance.

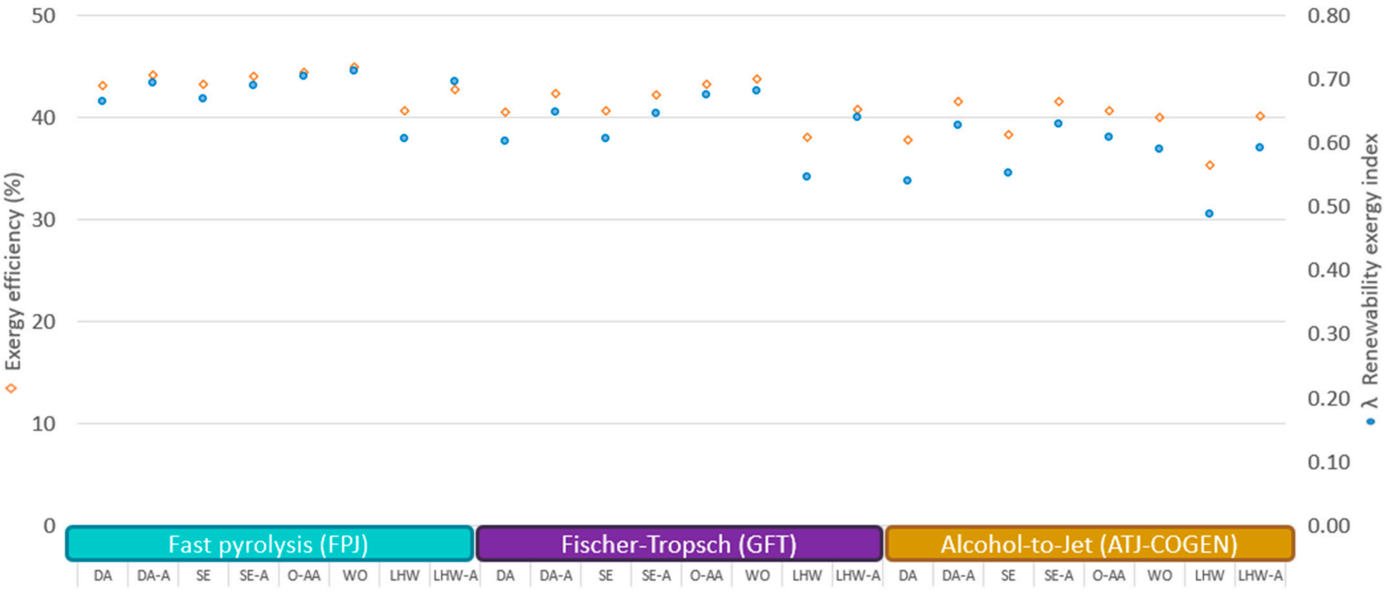


Figure 4. Exergy efficiency and the renewability index correlation for SAF production routes.

3.2. *Benchmark of Renewable Jet Fuel Conversion Routes*

In terms of biojet fuel production, when compared with the technologies based on integrating 1G and 1G–2G systems, the exergy performances of the hydrothermal liquefaction (HTL) processes using various catalysts such as water (H_2O), sodium carbonate (Na_2CO_3), and iron (Fe) show the higher efficiencies and renewability index, followed by the hydroprocessed esters and fatty acids, Fischer-Tropsch, and alcohol-to-jet systems. These comparisons were calculated based on the screening of the technologies/feasibility level. Thus, the accuracy range with a typical variation (L: −20% to −30%) in low ranges is determined by the function of the state of process technology and data availability. In addition, the bagasse and straw consumption varies between authors for each technological route, which contrasts the exergy efficiency against the AUEC and, consequently, the CO_2 emissions emitted in the atmosphere due to its operation and the exergy of the products for each scenario. Hence, the overall analysis was based on the fuel production rate and the surplus electricity available for sale to the grid as main products. The λ was defined according to Equation (7) within the exergy of the "fossil" (chemical and biochemical inputs), the exergy of products, the exergy associated with the CO_2 emissions, and the irreversibilities.

To summarize the main results investigated by Klein et al. [26], Tzanetis et al. [27], Santos et al. [6], Alves et al. [28], and Braz and Mariano [29], Figure 5 provides the technical parameters included in the comparison of these biomass-based routes. In general, these publications adopted a cradle-to-gate approach, which focuses the analysis on the production of fuels and biobased products and excludes their final use (carbon burned associated with planes' engines) and disposal/deactivation phases. Lastly, Figure 5 contrasts the renewable jet fuel conversion routes against the promising scenarios (top 3 pathways) determined by the selected KPIs in this study.

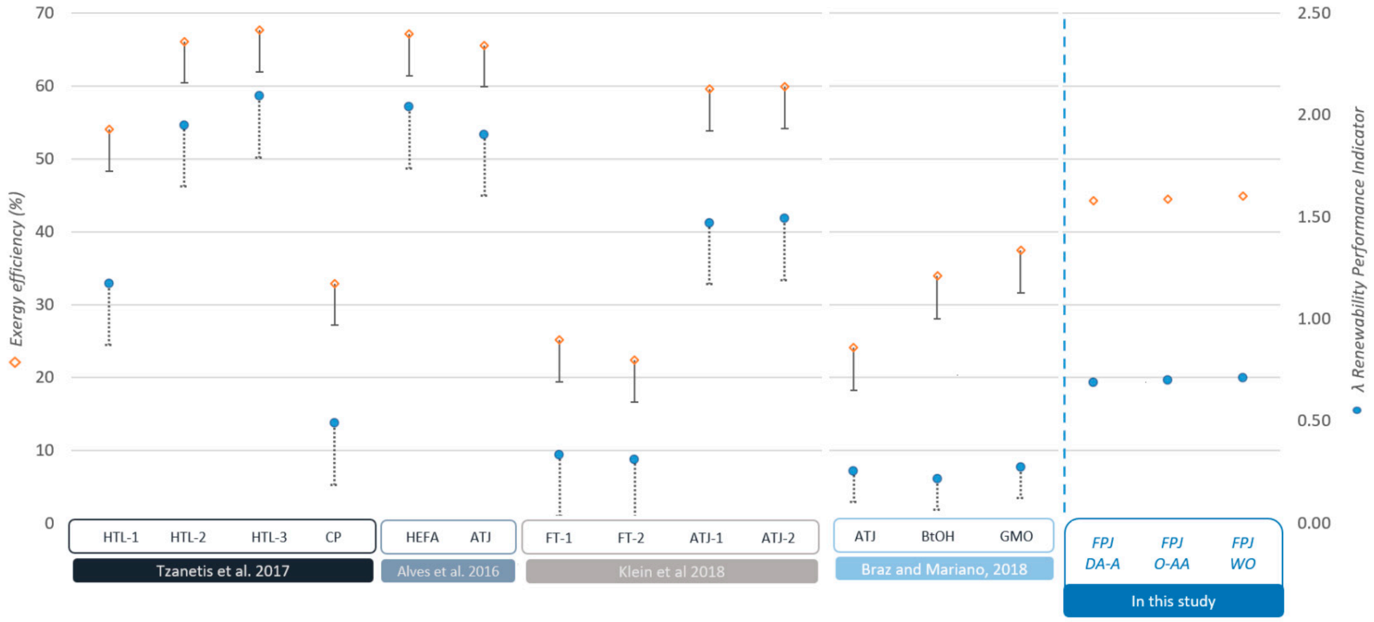


Figure 5. Benchmark of production pathways for renewable jet fuel. HTL represents hydrothermal liquefaction systems; catalytic pyrolysis (CP); alcohol-to-jet (ATJ); hydroprocessed esters and fatty acids (HEFA); and Fischer-Tropsch (FT) scenarios. BtOH denotes the Butanol Scenario, and GMO is the Butanol Scenario using genetically modified organisms [26–29].

4. Conclusions

The environmental impact and global performance of twenty-four promising biojet fuel routes were determined via a multi-criteria decision support analysis based on the selected KPIs to quantify the irreversibility and rank these technologies.

Concerning the exergy-based performance analysis, the λindex performs better for all pathways that use fast pyrolysis as a technology for lignin destination. Nonetheless, the exergy of the products could not be used to restore the environment to the conditions prior to the processing. The exergy assessment demonstrates that pre-treatment methods combined with the alkaline treatment (e.g., DA-A, SE-A, LHW-A) have a higher global performance than standalone lignocellulosic pre-treatments (e.g., DA, SE, O, WO, and LHW). The environmental performance applying the carbon dioxide equivalent indicator and the renewability exergy index as impact criteria shows that all pathways lead to a 30% reduction of specific CO_2 equivalent emissions in the exergy base compared to the conventional fossil-based jet fuels.

These insights on biomass-based fuels not only encourage further research in technology developments but also explore synergies across the competing biomass demand sectors (i.e., transport, heat, power, and biochemicals) to achieve competitiveness and significant potential for impact reduction regarding CO_2 and primary energy use based on a regulatory context (Brazilian framework, Renovabio), biomass availability, and conversion technologies conditions. For instance, the analysis could be extended to non-drop-in fuels (ICAO fuel categorization), which require changes to existing and legacy airframes and fueling infrastructure (i.e., liquefied gas aviation fuels, cryogenic hydrogen, and electricity); the analysis may also consider heat integration strategies in the integrated biorefinery systems and the addition of fuel use projections and the final use step (aircraft and engine combustion).

Finally, these types of KPIs based on thermodynamic principles could support certification processes and the regulation of international aviation emissions towards implementing regional market-based measures by country/area. Specific focus could be given to drop-in and non-drop-in fuels and deploying pathways, including emissions-trading systems such as the European Union Emissions Trading System (EU-ETS) and policies/regulations to promote (CORSIA) sustainable aviation fuels.

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Nomenclature

AUEC	Average unit exergy cost (kJ/kJ)
B	Exergy flow rate (kW)
b	Specific exergy (kJ/kg)
bch	Standard chemical exergy (kJ/kg)
c	Average unit exergy cost (kJ/kJ)
CO_{2EE}	Specific CO_2 equivalent emissions (*exergy base*) (kg/GJ)
CV	Control volume
I	Irreversibility rate (KW or MW)
h	Specific enthalpy (kJ/kg)
$\dot{m}$	Mass flow rate, (kg/s)
P	Pressure (kPa, bar)
$\dot{Q}$	Heat rate (kW)
s	Specific entropy (kJ/kg K)
t	Temperature, (°C, K)
$\dot{W}$	Power, (kW)
x	Mole or mass fraction
η_B	Exergy efficiency (%)

Abbreviations

ATJ	Alcohol-to-Jjet
DSHC	Direct Sugar to Hydrocarbon
CORSIA	Carbon Offsetting and Reduction Scheme for International Aviation
FT	Fischer-Tropsch
LCAF	Lower-Carbon Aviation Fuels
HDCJ	Hydrotreated Depolymerized Cellulosic Jet
HEFA	Hydroprocessed Esters and Fatty Acids
H_2SMR	Hydrogen Steam Methane Reforming
NREU	Non-Renewable Energy Use
GFT	Gasification Fischer-Tropsch
GHG	Greenhouse gas emissions
GWP	Global Warming Potential
SC	Sugarcane
PtL	Power-to-Liquid
WWT	Wastewater Treatment
WtWa	Well-to-Wake

Greek symbols

η	efficiency
λ	renewability exergy index

Appendix A

Table A1 presents the technical parameters of the milling process adopted in this study, whereas Table A2 shows the main parameters considered in the ethanol upgrade to jet process. Furthermore, Tables A3 and A4 display the operation parameters adopted in lignin fast pyrolysis and syngas Fischer-Tropsch, respectively. Lastly, Table A5 displays the key performance indicators for all the configurations analyzed and Table A6 gives the emission characterization factors and standard chemical exergy per resource.

Table A1. Operation parameters of the milling process.

Unit	Condition	Value	Units
Cleaning and crushing	Water make-up	0.05	m^3/TC *
	Fibers separation efficiency	100	%
	Bagasse moisture	53.8	%
	Imbibition water	0.28	ton/TC
	Imbibition water recycling	100	%
Liming settling and filtration	Sugars (sucrose, glucose) recovered	95	%
	Phosphoric Acid (H_3PO_4)	0.2	kg/ton SC
	Calcium oxide (CaO)	1	kg/TC
	Flocculant polymer	2.5	g/TC
	Fraction of soluble solids retained in filter	65	%
	Fraction of insoluble solids precipitated	99.7	%
	Washing water	8.19	kg/kg_{sugars}
Juice concentration	Pressure in 5th effect	0.16	bar
	Temperature in 1st effect	115	°C
	Juice solids content to sell	65	%
Juice solids content to fermentation	Defined in fermentation with constraints - final solids content $\leq$ 65 - Ethanol conc. end of fermentation $\leq$ 10%		

* TC: tons of cane; SC: Sugarcane. Adapted from [6,28].

Table A2. Operation parameters considered in ethanol upgrade to jet process.

Unit	Condition	Value
Pump	ΔP (bar)	4
Dehydration reactor	P (bar)0/T (°C)	4/375
	Catalyst used	Heterogeneous, 0.5%La–2%P H-ZSM-5
	Reactor specifications	Multi-tubular fixed bed in a furnace
Decanter (Fraction of components in the gas outlet)	Water ethylene	1.16% 100%
Compressor	ΔP (bar)	30
Oligomerization reactor butylene synthesis	P (bar)/T (°C)	30/200
Oligomerization reactorbutylene oligomerization	P (bar)/T (°C)	89/200
Oligomerization general	Catalyst	Ziegler Natta-type
	Reactor type	Fixed bed
Compressor of H_2	ΔP (bar)	30
Hydrogenation reactor and decanter	P (bar)/T (°C)	30/250
	Catalyst	palladium and platinum over GAC
	WHSV (h^{-1}) w/w	3
	Lifetime (years)	5
	H_2 requirement (kg/kg olefins)	0.05
	H_2 excess	50% of the amount reacted
Steam distillation	Live steam required (kg/kg paraffin)	0.258
	Fraction of compounds in LPG stream	
	LPG Naphtha Water	97% 32% 2.38%
	Fraction of compounds in naphtha stream	
	LPG Naphtha Water	3% 62% 0.01%

Adapted from [6,28].

Table A3. Operation parameters considered in lignin fast pyrolysis.

Unit	Condition	Value
Lignin dryer	Max. lignin moisture	8%
	T final (°C) FPJ	307
	Air make-up (kg air/kg water evaporated)	2.605
Lignin grinder	Diameter of lignin particles (mm)	≈2
Fast pyrolysis fluidized auger bed	P (bar)/T (°C)/Residence time (s)	1.5/500/2
	Sand/biomass (kg/kg)	14.5
	Fluidization gas/lignin (kg/wet kg lignin)	3

Table A3. *Cont.*

Unit	**Condition**	**Value**
Cyclone	Solid/gas separation efficiency	100%
Quenching column	Chilled water/inlet stream (kg/kg)	1.445
	Fraction of components in the bio-oil stream	
	Phenolics (organic liquid fraction bio-oil) Light ends Water Non-condensable compounds	100% 49.34% 45.06% 0%
Sand heater/Char combustor	T of gas and sand (°C)	608
	O_2 excess (kgO_2/kgO_2 consumed in char combustion)	1.2

Adapted from [6,28].

Table A4. Operation parameters adopted in syngas Fischer-Tropsch.

Unit	**Condition**	**Value**
Syngas polishing	P (bar)/T (°C)	25/150
	Packing/lignin flowrate (kg/kg dry lignin/day)	0.853
	Max. H_2S concentration (kg/kg clean syngas)	5.0×10^{-8}
	Max. NH_3 concentration (kg/kg clean syngas)	1.0×10^{-5}
H_2 SMR	P (bar)/T (°C)	25/870
	Catalyst	Ni and aluminum
	Catalyst/H_2 synthesized flowrate (kg/kg H_2/day)	0.058
	HP steam/CH_4 inlet (mol/mol)	6
	CH_4 concentration in the outlet (%)	1.5
	T outlet (°C) of cooling water	300
Water gas shift	Catalyst	Copper-zinc
	Catalyst/lignin flowrate (kg/kg/day)	0.00297
PSA	H_2 recovery efficiency/Purity (%)	85/100
	Packing	2/3 with activated carbon and 1/3 with molecular sieve
	H_2/carbon compounds in PSA outlet (mass %)	0.0136
FT reactor	P (bar)/T (°C)	25/200
	Catalyst	Cobalt on AlO_3
	Catalyst/lignin flowrate (kg/kg/day)	0.0926
Separator/Decanter	Water/gas/organic phase separation efficiency	100%
Hydroprocessing	H_2 requirement$_{\text{minimum}}$ (kg H_2/kg waxes)	0.06

Adapted from [6,28].

Table A5. Key performance indicators for each biorefinery configuration.

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
pre-treatment	*DA*	*DA*	*DA*	*DA*	*DA*	*DA*	*DA*	*DA*	*DA*
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	43.16	40.55	37.88	20.63	19.54	15.54	22.15	19.14	16.22
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	91,041	85,540	79,881	43,522	41,216	32,783	46,716	40,375	34,212
I (KW)	119,084	124,573	130,264	166,609	168,903	177,371	163,424	169,753	175,952
AUEC (kJ/kJ)	2.32	2.47	2.64	4.85	5.12	6.43	4.51	5.22	6.16

	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
pre-treatment	*DA-A*	*DA-A*	*DA-A*	*DA-A*	*DA-A*	*DA-A*	*DA-A*	*DA-A*	*DA-A*
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	44.22	42.37	41.64	19.44	17.59	16.86	19.44	17.60	16.86
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	93,282	89,383	87,827	41,011	37,113	35,557	41,011	37,113	35,557
I (KW)	116,831	120,726	122,296	169,109	173,005	174,575	169,119	173,014	174,585
AUEC (kJ/kJ)	2.26	2.36	2.40	5.14	5.68	5.93	5.14	5.68	5.93

	19	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**
pre-treatment	SE	SE	SE	SE	SE	SE	SE	SE	SE
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	43.25	40.69	38.37	20.43	17.87	15.55	20.43	17.88	15.55
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	91,215	85,825	80,910	43,088	37,698	32,783	43,088	37,698	32,783
I (KW)	118,937	124,314	129,262	167,072	172,449	177,397	167,081	172,459	177,407
AUEC (kJ/kJ)	2.31	2.46	2.61	4.89	5.59	6.43	4.89	5.59	6.43

	28	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**
pre-treatment	SE-A	SE-A	SE-A	SE-A	SE-A	SE-A	SE-A	SE-A	SE-A
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	44.00	42.30	41.64	19.22	17.52	16.86	19.22	17.52	16.86
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	92,806	89,222	87,827	40,536	36,951	35,557	40,536	36,951	35,557
I (KW)	117,323	120,904	122,312	169,602	173,183	174,591	169,608	173,189	174,596
AUEC (kJ/kJ)	2.27	2.36	2.40	5.20	5.71	5.93	5.20	5.71	5.93

	37	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**
pre-treatment	O-AA	O-AA	O-AA	O-AA	O-AA	O-AA	O-AA	O-AA	O-AA
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	44.43	43.29	40.65	20.24	19.10	16.46	20.24	19.10	16.46
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	93,751	91,347	85,765	42,702	40,298	34,716	42,702	40,298	34,716
I (KW)	116,310	118,701	124,313	167,366	169,757	175,369	167,376	169,767	175,379
AUEC (kJ/kJ)	2.25	2.31	2.46	4.94	5.24	6.08	4.94	5.24	6.08

	46	**47**	**48**	**49**	**50**	**51**	**52**	**53**	**54**
pre-treatment	O-GAC	O-GAC	O-GAC	O-GAC	O-GAC	O-GAC	O-GAC	O-GAC	O-GAC
technology	*ATJ*	*ATJ*	*ATJ*	*DFJ*	*DFJ*	*DFJ*	*DFJ-DA*	*DFJ-DA*	*DFJ-DA*
lignin destination	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*	*FPJ*	*GFT*	*cogen*
η_B (%)	44.44	43.29	40.65	20.24	19.10	16.46	20.24	19.10	16.46
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	93,751	91,347	85,765	42,702	40,298	34,716	42,702	40,298	34,716
I (KW)	116,320	118,711	124,323	167,375	169,766	175,378	167,385	169,776	175,387
AUEC (kJ/kJ)	2.25	2.31	2.46	4.94	5.24	6.08	4.94	5.24	6.08

Table A5. *Cont.*

	55	**56**	**57**	**58**	**59**	**60**	**61**	**62**	**63**
pre-treatment technology lignin destination	*WO* *ATJ* *FPJ*	*WO* *ATJ* *GFT*	*WO* *ATJ* *cogen*	*WO* *DFJ* *FPJ*	*WO* *DFJ* *GFT*	*WO* *DFJ* *cogen*	*WO* *DFJ-DA* *FPJ*	*WO* *DFJ-DA* *GFT*	*WO* *DFJ-DA* *cogen*
η_B (%)	44.94	43.79	40.02	21.15	19.99	16.22	21.15	20.00	16.22
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	94,808	92,370	84,408	44,612	42,174	34,212	44,612	42,174	34,212
I (KW)	115,286	117,749	125,743	165,527	167,954	175,948	165,537	167,963	175,958
AUEC (kJ/kJ)	2.23	2.28	2.50	4.73	5.00	6.16	4.73	5.00	6.16
	64	**65**	**66**	**67**	**68**	**69**	**70**	**71**	**72**
pre-treatment technology lignin destination	LHW *ATJ* *FPJ*	LHW *ATJ* *GFT*	LHW *ATJ* *cogen*	LHW *DFJ* *FPJ*	LHW *DFJ* *GFT*	LHW *DFJ* *cogen*	LHW *DFJ-DA* *FPJ*	LHW *DFJ-DA* *GFT*	LHW *DFJ-DA* *cogen*
η_B (%)	40.72	38.13	35.38	32.90	30.31	27.56	32.90	30.31	27.56
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	85,884	80,430	74,629	69,389	63,935	58,133	69,389	63,935	58,133
I (KW)	124,231	129,671	135,508	140,733	146,174	152,011	140,742	146,183	152,020
AUEC (kJ/kJ)	2.46	2.62	2.83	3.04	3.30	3.63	3.04	3.30	3.63
	73	**74**	**75**	**76**	**77**	**78**	**79**	**80**	**81**
pre-treatment technology lignin destination	LHW-A *ATJ* *FPJ*	LHW-A *ATJ* *GFT*	LHW-A *ATJ* *cogen*	LHW-A *DFJ* *FPJ*	LHW-A *DFJ* *GFT*	LHW-A *DFJ* *cogen*	LHW-A *DFJ-DA* *FPJ*	LHW-A *DFJ-DA* *GFT*	LHW-A *DFJ-DA* *cogen*
η_B (%)	42.70	40.86	40.13	18.80	16.95	16.22	18.80	16.95	16.22
B_{inputs} (KW)	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525	210,525
$B_{outputs}$ (KW)	90,085	86,197	84,647	39,649	35,762	34,212	39,649	35,762	34,212
I (KW)	120,014	123,898	125,463	170,459	174,343	175,908	170,469	174,353	175,917
AUEC (kJ/kJ)	2.34	2.45	2.49	5.32	5.90	6.17	5.32	5.90	6.17

TECHNOLOGIES: ATJ: Alcohol-to-Jet (fermentation); COGEN: Cogeneration; DFJ: Direct fermentation via farnesene; FPJ: Fast pyrolysis; GFT: Gasification Fischer-Tropsch. *PRE-TREATMENTS:* DA: Dilute-acid; DA-A: Dilute acid + alkaline treatment; SE: SO_2 steam explosion; SE-A: Steam explosion + alkaline treatment; O: Organosolv; O-GAC: Organosolv + Granular activated carbon adsorption; WO: Alkaline wet oxidation; LHW: Liquid hot water; LHW-A: Liquid hot water + alkaline treatment.

Table A6. GHG emission characterization factors and standard chemical exergy per resource.

	Resources (x)	**Input/ Output** $^+$	**GHG (kg_{CO2}/x)**	**Units (x)**	**Notes**	**b_{CH} (kJ/kmol)**	**b_{CH} (MJ/kg)**
From Ecosphere (environment)	Sugarcane *	input	0.034	kg	Including transportation, without trash burning, with sugar yield of our process	-	5.13
	SC bagasse *	input	0.01	kg	Using the yield of sugars, of sugarcane bagasse/sugarcane	-	9.67
	Enzyme *	input	4.09	kg	kg of enzyme ($CH_{1.57}N_{0.29}O_{0.31}S_{0.007}$)	541,376	23.73 ^{A}
	Water **	input	0.002	kg	Estimated from the electricity of a cooling pump with 80% efficiency to cool down 1 kg of chilled water	900	0.05

Table A6. *Cont.*

	Resources (x)	Input/ Output +	GHG (kg_{CO2}/x)	Units (x)	Notes	b_{CH} (kJ/kmol)	b_{CH} (MJ/kg)
Chemicals and others	$(CH_3)_2CO$ **	difference between input and output	2.19	kg	Acetone liquid	1,788,500	30.85
	$C_2H_4O_2$ **	input	1.403	kg	Acetic acid via methanol carbonylation	908,000	15.30
	CaO **	input	0.15	kg	Lime (100%)	110,200	1.97
	$C_{10}H_{14}O_2$	input	3.163	kg	kg CO_2/kg tert-butyl catechol produced from lignin	5,049,720	30.42 ^{B}
	Na_2CO_3 **	input	0.59	kg	Sodium carbonate (caustic soda), 50%, Na_2CO_3	41,100	0.39
	NaOH **	input	1.096	kg	Analyzing 1 kg 'Sodium hydroxide, 50% in H_2O, production mix, at plant/RER U'	74,900	1.87
	NH_4OH **	input	2.089	kg	Ammonia, liquid, at regional storehouse/kg/RER	337,900	19.84
	H_3PO_4 **	input	1.423	kg	Commercial phosphoric acid (15%) used has a concentration of 85% by mass	89,600	0.91
	H_2SO_4 **	input	0.124	kg	Sulfuric acid	163,400	1.67
	SO_2 **	input	0.44	kg	Sulfur dioxide, liquid	313,400	4.89
	Waste to landfill	output end life	0.329	kg	Disposal, average incineration residue, 0% water, to residual material landfill	-	-
Electricity and Fuels	Electricity	input	0.486	kWh	Electricity, production mix RER/kWh/RER	-	-
	Natural gas	input	1.422	kg	Emissions in production from fossil fuels (extraction, transportation, and processing)	829,457	51.70 ^{C}
	Natural gas (emissions)	output	2.284	kg	Combustion of CH_4 emissions	-	-
	Liquefied petroleum gas (LPG)	input	2.871/0.139	kg	Combustion emissions/extraction and processing of LPG, which typically consists of propane (C_3H_8) or a mixture of propane and butane (C_4H_{10})	2,483,915	45.01 ^{C}
	Gasoline (C_8H_{18})	input	2.789/0.503	kg	Emissions in utilization and production from fossil fuels	5,413,532	47.39 ^{C}
	Diesel ($C_{12}H_{23}$)	input	2.966/0.568	kg	Emissions in utilization and production from fossil fuels	7,130,900	42.70 ^{D}
	Jet fuel (transportation)	output	4.5/17.1	t.km	São Paulo, by train (150 km), Rio de Janeiro, by train (570 km)	7,565,100	45.30 ^{D}

+ The main inventories of this section are based on Santos et al. [6]. * Calculated using the correlations linking the ratio of the standard chemical exergy (b_{CH}) and the net calorific value of the substances [30]. ** Adopted values for b_{CHspec} from Szargut et al. [9]. ^{A} For the enzymes, the composition ($CH_{1.57}N_{0.29}O_{0.31}S_{0.007}$) indicated per NREL was assumed [31]. ^{B} Predicted based on the correlations between the high heating value of the fuel and the chemical exergy of the combustion products (net heat of combustion) [32]. ^{C} Based on values and composition reported by Arango-Miranda et al. [33]. ^{D} Based on reference values given in Dincer and Rosen [34].

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