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**TÍTULO DO TRABALHO:**

TECHNICAL ASSESSMENT OF FISCHER-TROPSCH LIQUID FUEL PRODUCTION THROUGH GASIFICATION OF SUGARCANE BAGASSE AND STRAW IN THE BRAZILIAN BIOFUELS INDUSTRY

**AUTORES:**

Mateus Henrique Rocha
Marcelo José Colaço
Albino José Kalab Leiroz

**INSTITUIÇÃO:**

Universidade Federal do Rio de Janeiro

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## Abstract

This work investigates the potential of using sugarcane bagasse and straw in thermochemical processes to produce renewable energy. By focusing on the gasification processes, this study evaluates the bioenergy potential of sugarcane residues as a sustainable alternative to fossil fuels. Key process parameters were calculated to optimize the energy conversion process. It was demonstrated that the sugarcane bagasse and straw are suitable feedstocks for producing syngas with a high hydrogen and carbon monoxide content. Additionally, the potential integration of these processes into existing biofuel production systems in Brazil is discussed, aiming at improving the energy efficiency of sugarcane biorefineries. The study contributes to the broader goals of reducing greenhouse gas emissions and increasing the use of renewable energy sources in the country's energy matrix. In this work, it was considered that the amount of biomass available from just one plant would be insufficient to produce a reasonable and sufficient quantity of fuels. Therefore, a cluster containing four associated plants was conceived. The biomass would be transported within a radius of no more than 100 km to the site of the thermochemical conversion plant. The new biorefinery configuration would be capable of processing 110.8 kg/s of biomass, producing 3.0 kg/s of gasoline and 7.09 kg/s of diesel, and exporting 53.80 MW of electricity to the grid. The overall efficiency of the newly conceived process is 47.0%.


**Keywords: sugarcane bagasse, straw, thermochemical process, gasification, synthesis gas, Fischer-Tropsch synthesis, gasoline, diesel, power generation**

## 1) Introduction

Several researchers have been working on the process synthesis and design of large-scale biorefinery systems, including Klüh et al. (2024) and Piazzi et al. (2022), who carried out technical assessments of the production of methanol, mixed alcohols, hydrogen ($H_2$), urea, Fischer-Tropsch Liquids (FTL) (diesel, gasoline, and jet fuel), and electricity from biomass, but only at different production ratios. These works analyzed the material, mass, and carbon balances, thermodynamic performance evaluation, unit operations energy consumption, and overall efficiency of biorefineries using specific process simulation software. Additionally, addressed the detailed economic cost analysis (capital and production costs) of the best technology for different biomass-to-liquid production plants based on the thermochemical route. The main focus of these works was to analyze the liquid fuels production via catalytic synthesis with electricity as a co-product using commercial technology available for implementation within the next 5-10 years.

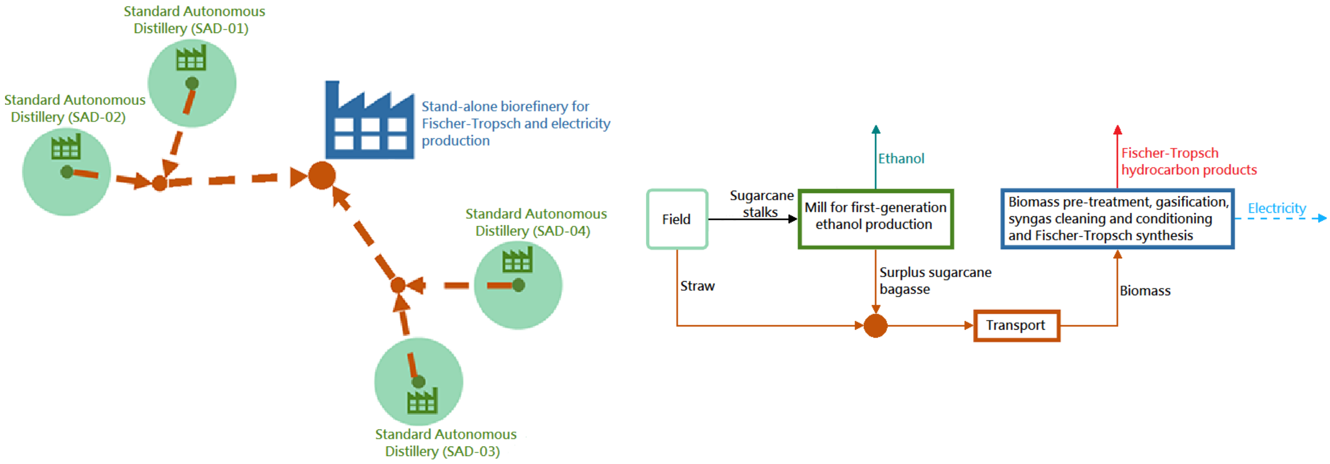
This research focuses on producing renewable transportation fuels from biorefineries based on sugarcane bagasse and straw gasification. This study introduces a novel approach to produce transportation liquid fuels such as syncrude (liquid hydrocarbons) such as diesel and gasoline through thermochemical processes. This method integrates biomass gasification with synthesis gas (syngas) cleaning, conditioning, and fuel synthesis and upgrading, facilitating the production of new biofuels from biomass. In this study, the Aspen Plus™ software was used for process modeling and calculations to solve material and energy balances. An Aspen Plus™ process flowsheet model of biorefinery systems was developed to analyze these systems and generate energy and mass balances for different biorefinery configurations. Additionally, a chemical equilibrium model was employed to assess fuel production scenarios, using gasification equilibrium results to model fuel production and evaluate the impacts of analyzed parameters.

## 2) Methodology

In order to evaluate the performance of a Stand-Alone Biorefinery (SAB) system for producing Fischer-Tropsch (FT) hydrocarbon products and electricity, different scenarios were proposed using Aspen Plus™ software, a widely used commercial process simulator for modelling, design, and process optimization in a steady-state environment. The biorefinery is represented by a SAB plant consisting of an independent, self-contained biomass-to-liquid facility. The SAB could potentially be implemented in existing Standard Autonomous Distilleries (SADs) currently operating in Brazil.

The surplus sugarcane bagasse could be utilized as raw material in the designed biorefinery. The most of sugarcane bagasse is used as fuel in power plants for first-generation ethanol production. It is necessary to evaluate the availability of the straw, its quality, recovery routes, related costs, agronomic impacts, environmental impacts, and final use for power generation in advanced systems. Literature reports indicate that 30% to 60% of the straw could be recovered in an economically feasible manner (Fioranelli and Bizzo, 2023).

In this study, it is assumed that 50% of the straw available in the field will be recovered and transported to the standard autonomous distillery to be used as feedstock in the biorefinery. The total amount of straw available in the field is 140 kg (dry basis) per ton of sugarcane (tc) stalks. The straw represents one of the largest truly sustainable feedstock potentials that can be utilized in the short to medium term. Given that the biorefinery concept requires a large amount of biomass feedstock, the technical assessment was conducted for 4 SADs operating jointly in a cluster format (as shown in **Figure 1**), aiming to achieve the minimum required syngas quantity to obtain an economically competitive scale factor, as reported by Sudiro and Bertucco (2009). **Table 1** presents the basic parameters considered in each SAD evaluated in this work and **Table 2** presents the energy balance of each SAD and the biomass availability for the FTL production.




(a) (b)

Figure 1 – Overview of the spatial configuration of the stand-alone biorefinery for Fischer-Tropsch syncrude and electricity production.

Table 1 – General characteristics of the standard autonomous distillery adopted in the simulation (Palacios-Bereche et al., 2013).

| Parameters | Unit | Value |
|---|---|---|
| Milling capacity | ton/h | 500 |
| Sugarcane crushed per harvest season | ton/season | 2,160,000 |
| Sugarcane productivity | ton/ha | 82.4 |
| Effective operating hours | h/year | 4320 |
| Sugarcane bagasse availability | kg bagasse/tc | 240 |
| Straw availability | kg straw/tc | 140 |
| Ethanol production yield | l/tc | 91.0 |
| Electric power demand of first-generation ethanol production | kWh/tc | 12.0 |
| Mechanical power demand of first-generation ethanol production | kWh/tc | 16.0 |

Table 2 – Description of the evaluated scenarios.

| Parameters | Unit | Values (Dias et al., 2011) |
|---|---|---|
| Steam pressure of the distillery | MPa | 8.0 |
| Steam temperature of the distillery | ºC | 510 |
| Steam consumption of the distillery | kg steam/tc | 226 |
| Surplus of electricity | kWh/tc | 7.0 |
| Surplus of sugarcane bagasse | % | 54.0 |
| Straw availability in the field | kg/tc | 140 |
| Sugarcane bagasse stream flow rate | kg/s | 18.0 |
| Straw stream flow rate | kg/s | 9.72 |
| Total biomass available flow rate | kg/s | 27.72 |

There are two ways to simulate the process of producing hydrocarbon fuels through FT synthesis: Once-Through (OT) design (Open Loop Cycle) and Recycle (RC) design (Closed Loop Cycle). In this work, the single-pass OT design was chosen because it allows for the recovery of thermal energy from the process for the export of power to the grid, as shown in Figure 2. In the OT configuration, the syngas passes through the FT synthesis reactor only once, so the unreacted off-gas, with a significant unconverted syngas fraction, is used as fuel gas for a steam turbine for power generation. The hot exhaust of the turbine is used, together with waste heat recovered from various places in the process, to raise steam to drive a steam turbine. The power generated by the gas turbine and steam turbine combined cycle is sufficient to provide the power needed to operate the plant, plus a significant amount of power for export to the grid. As a result, the systems are able to meet all the electricity needs and export power to the grid. The large amount of electricity produced suggests labeling the electricity as a co-product rather than a by-product (Selvatico et al., 2016).

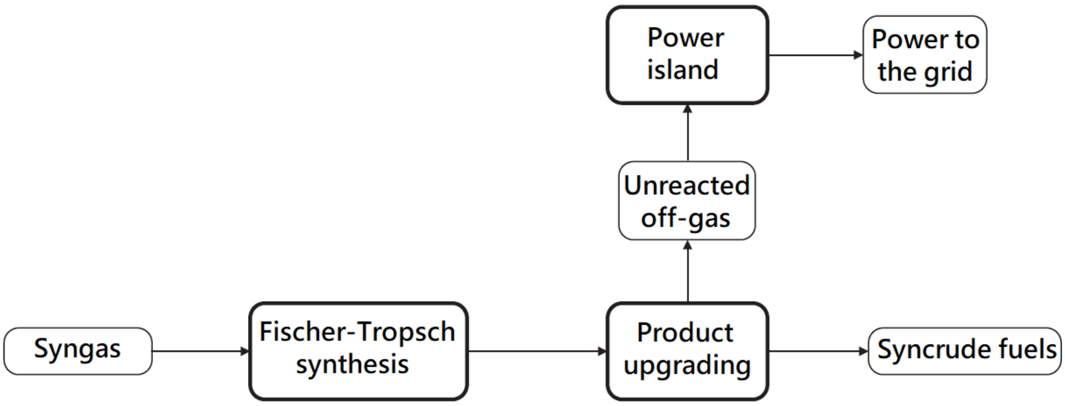



Figure 2 – FT configuration selected in this work.

At the end of the drying process, the moisture content of the biomass is set to be 10%. Sugarcane bagasse and straw are defined as non-conventional components in Aspen Plus™ from their respective ultimate analysis, proximate analysis, and the particle size distribution, as shown in Table 3.

Table 3 – Characteristics of sugarcane bagasse and straw used in this analysis.

| Parameters | Unit | Bagasse (Hassuani et al., 2005) | Straw (Seabra et al., 2010) | ABNT standard | Aperture size of sieve (mm) | Bagasse (Hassuani et al., 2005) | Straw (Seabra et al., 2010) |
|---|---|---|---|---|---|---|---|
| Proximate analysis | | | | 3.5 | 4.80 | 6.455 | 0 |
| Moisture content | % d.b. | 50.2 | 15.0 | 7 | 2.40 | 9.655 | 38.96 |
| Ash | % d.b. | 2.25 | 3.9 | 16 | 1.20 | 12.895 | 7.48 |
| Fixed carbon | % d.b. | 18.0 | 12.8 | 30 | 0.60 | 31.625 | 18.50 |
| Volatile matter | % d.b. | 79.9 | 83.3 | 50 | 0.30 | 25.825 | 22.98 |
| Ultimate analysis | | | | 100 | 0.15 | 11.255 | 0 |
| Carbon | % d.b. | 45.59 | 46.1 | Bottom | <0.15 | 2.290 | 12.08 |
| Hydrogen | % d.b. | 5.93 | 6.2 | Sum | ---- | 100 | 100 |
| Nitrogen | % d.b. | 0.61 | 0.60 | Heats of combustion | | | |
| Oxygen | % d.b. | 45.49 | 43.08 | Lower Heating Value (LHV) | MJ/kg | 7.52 | 13.30 |
| Sulfur | % d.b. | 0.11 | 0.10 | Higher Heating Value (HHV) | MJ/kg | 18.10 | 17.40 |
| Chlorine | % d.b. | 0.02 | 0.02 | **d.b.: dry basis** | | | |

A process flowsheet is generated in Aspen Plus™ consisting of seven key unit operations. The biorefinery process is divided into seven major technical Areas, as shown in Figure 3. A variety of technologies were considered for this study including entrained flow gasification, syngas cleaning techniques and low temperature FT synthesis without syngas recycle.

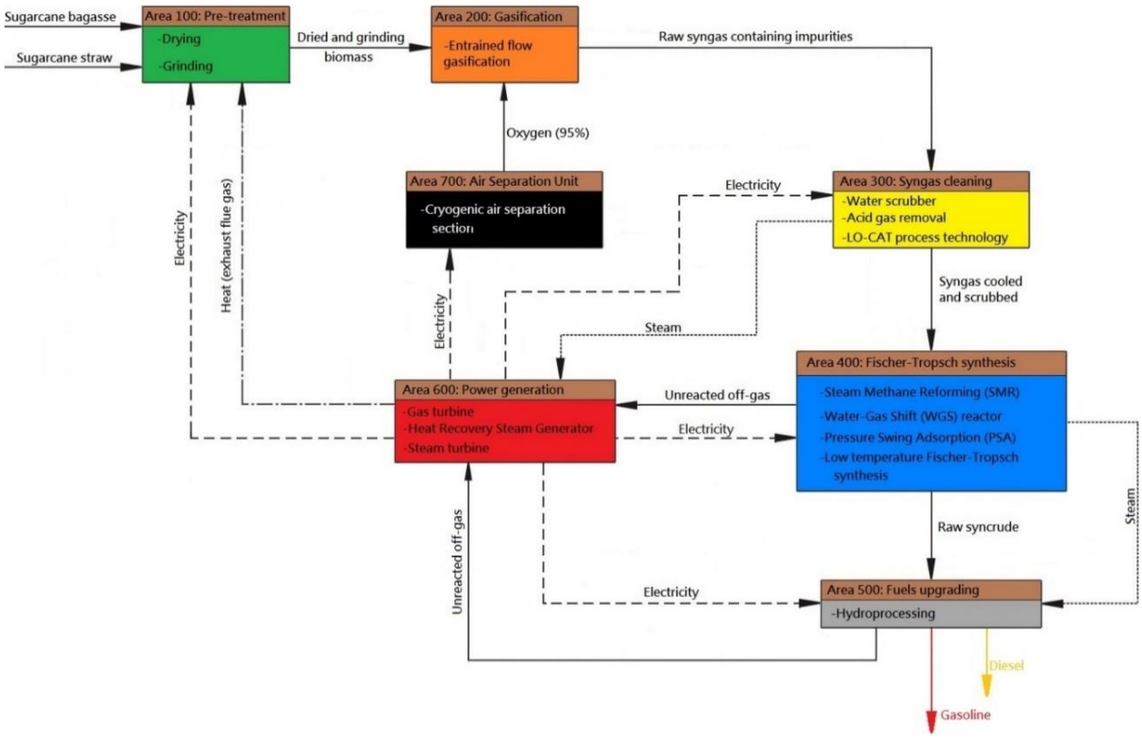



Figure 3 – Overall process flow diagram for the scenario evaluated in this work.

- **Area 100:** pre-treatment that consists of drying and grinding. Wet biomass stream is introduced into the stoichiometric reactor with hot flue gas at temperature of 250ºC. This reactor operates at atmospheric pressure (101.325 kPa) and the heat loss is assumed to be zero because it is assumed that the drying is an adiabatic process. It is assumed that the electric power consumption for the drying step is set to 115 kJ/kg dry biomass for the operation of the blower and transportation system (Tuomi et al., 2019). It is considered that the latent heat of evaporation will be used to calculate the flow rate of the hot flue gas, which will be used for drying the biomass. The latent heat was assumed to be constant and equal to 2501.30 kJ/kg (Perazzini et al., 2021). In this work, it will be considered that the specific energy consumption for biomass size reduction is 75 kWh/ton, a value reported by Karinkanta et al. (2018), who ground wood to a particle size of 350 μm.

- **Area 200:** biomass gasification evaluated based on chemical equilibrium calculations. The Aspen Plus™ reactor models used in this work are the single-phase chemical equilibrium model or simultaneous phase and chemical equilibrium model. Gibbs free energy minimization is performed to determine the product composition. The following assumptions were made for the simulation of biomass gasification, as reported by Násner et al. (2017): gasification process is in steady state; the gasification zone is completely isothermal; pressure and temperature are uniform inside the gasifier (in all directions: axial and radial); residence time is sufficiently long enough to allow the chemical reactions to reach the equilibrium state; reactor hydrodynamic characteristics are not considered; the average particle diameter remains constant during gasification; char is composed only of carbon and ashes; tar compounds are not considered; and all of the sulfur and chlorine compounds will react to form $H_2S$ and HCl. To determine the thermodynamic properties of the components in the process reactions, the Aspen Plus™ software has several predetermined models. Peng-Robinson with Boston-Mathias function (PR-BM) was selected for the gasification process (Martelli et al., 2011; Meerman et al., 2011).

- **Area 300:** the direct quench syngas cooling occurs, removing fly ash and tars in the form of sludge and black water to limit downstream plugging. The direct water quench reduces the syngas temperature to approximately 40 °C after the scrubber to condense the tars and also collect $NH_3$ and $NH_4Cl$, which dissolve in water. The wet scrubber was modeled with a Venturi scrubber gas-solid separator (VScrub) coupled with a gas-liquid separator (Sep), respectively, as indicated by Aguado et al. (2023). The syngas then entered a wet scrubber, which was simulated as a separator where 99% of the ammonia and 95.8% of the tar were removed in the exhaust stream. The wet scrubber required a lot of water for its operation (1.20 liters $H_2O$/kg raw syngas); therefore, to limit this consumption, the stream was partly recirculated. Otherwise, the purged fraction was sent to water treatment (Regis et al., 2023). In this study, a 20% concentrated MEA, which absorbs 0.4 moles of acid gas/mole of MEA, is used as the absorbent. The $H_2S$ exits the top of the absorber at 4 ppm, and $CO_2$ exits at 2%, corresponding to 99% and 90% removal, respectively. The clean syngas is then ready for polishing to meet final cleanliness requirements. The acid gas is directed to the LO-CAT™ sulfur recovery system to isolate the $H_2S$ and convert it to solid sulfur. The LO-CAT™ system uses $O_2$ and a liquid solution of $Fe^{+3}$ to oxidize $H_2S$ to elemental sulfur (Swanson et al., 2010).

- **Area 400:** the key processes in this area include ZnO and activated carbon gas polishing, syngas booster compression, Steam Methane Reforming (SMR), Water-Gas Shift (WGS), $H_2$ separation via Pressure Swing Adsorption (PSA), FT synthesis, FT product separation, and unconverted syngas distribution. According to Santos and Alencar (2020), the syngas entering the FT synthesis must have contaminant levels below 200 ppb of sulfur and 10 ppm of $NH_3$. As sulfur concentrations at this stage of the process exceed the allowable limits, the syngas undergoes a polishing step using a ZnO and activated carbon sorbent to remove sulfur and trace contaminants. Following this, because FT synthesis requires an operating pressure of 25 bar and the incoming syngas is at approximately 22 bar, the syngas stream is compressed. Due to the significant amounts of $CH_4$ and $C_2H_6$ present in the syngas stream in the evaluated scenario, a SMR operating at equilibrium and 870 ºC is employed to reduce the accumulation of these components through recycle streams (Tuomi et al., 2019; Meerman et al., 2011). The WGS is positioned here to adjust the $H_2/CO$ syngas molar ratio, ensuring it slightly exceeds the optimal value for FT synthesis. A portion of the syngas is diverted to a PSA process to supply $H_2$ for the hydroprocessing section. The syngas reacts over a Co-based catalyst in a fixed-bed FT reactor at 200 ºC, with an assumed CO conversion rate of 40% per pass. The FT product distribution is modeled using the Anderson-Schulz-Flory (ASF) alpha chain growth mechanism, aiming for maximum yields of diesel and high molecular weight waxes by operating at an alpha value of 0.90 (Rafati et al., 2017).

- **Area 500:** through hydroprocessing, syncrude is converted into a product with properties comparable to petroleum-based fuels. The hydroprocessing model includes a distillation process that separates the hydrocarbons into two streams: one in the gasoline range and the other in the diesel range. Both streams are assumed to be suitable for blending into finished fuel without further refining. FTL contain significant amounts of waxes, are hydrocracked in a hydroprocessing unit. This area was not modeled in detail; instead, product distribution estimates were based on data from Furimsky (2013). $H_2$ required for the process is supplied from the fuel synthesis area and recycled within Area 500 as needed. The product distribution by weight from Area 500 is approximately 26% naphtha and 62% diesel, with the remaining portion consisting of gaseous hydrocarbons, which are used as fuel in a gas turbine. The resulting liquid fuels can then be blended into the gasoline and diesel storage tanks.
- **Area 600:** this section is responsible for the generation of thermal and electrical energy for the biorefinery, which is achieved through the unreacted off-gas from the FT synthesis and hydroprocessing units.

- **Area 700:** cryogenic Air Separation Unit (ASU) to supply $O_2$ (95%) used in biomass gasification). A two-column cryogenic $O_2/N_2$ separation system is employed with subsequent $O_2$ compression and $N_2$ vent. The ASU was not modeled in Aspen Plus™ software either, but the specific work consumption for delivering an oxygen stream at atmospheric pressure is 0.35 kWh/kg, which was included in the calculations. Additional work is required for further compression of the oxygen stream up to the desired process pressure, which is evaluated as 0.10 kWh/kg. Therefore, the estimated total specific work consumption is 0.45 KWh/kg (Kanbur et al, 2017).

## 3) Results and discussion

The overall mass balance including all process steps for the evaluated scenario is shown in the Figure 4. It should be noted that the energy integration of each of the four SAD with the central designed biorefinery was not included in the balance. The overall energy balance is shown in the Table 4. Considering 4320 hours of plant operation per year (harvest season), it would be possible to produce 46.656 kton/year of gasoline (60,592 $m^3$ gasoline/year) and 110.264 kton of diesel (129,722 $m^3$ diesel/year). To give an idea of the size of the biorefinery designed in this work, according to data from Petrobras, the largest refinery in Brazil is the Paulínia Refinery (REPLAN), which has the capacity to process 69,000 $m^3$ of crude oil per day and produce about 17 million liters of gasoline per day (66.205 million $m^3$ per year) and 24 million liters of diesel per day (8.76 million $m^3$ per year). The smallest refinery in Brazil is the Lubrificante e Derivados de Petróleo do Nordeste Refinery (LUBNOR), which produces around 250,000 liters of gasoline per day (91,250 $m^3$ per year) and 764,000 liters of diesel per day (278,860 $m^3$ per year). Therefore, the biorefinery designed in this work would be capable of producing around 66% of the total gasoline produced by the smallest Brazilian refinery currently, and approximately 47% of the total diesel fuel produced by the smallest Brazilian refinery.

As previously reported, each SAD is capable of producing 91.0 l of ethanol/tc, and each hectare planted with sugarcane is capable of producing 218.4 l ethanol/ha. In the new biorefinery configuration designed in this work, it would be possible to produce 7.1 l of gasoline/tc (585.04 l of gasoline/ha) and 15.1 l of diesel/tc (1244.24 l of diesel/ha). A comprehensive comparison of different biofuel supply routes uses energy efficiency as one key indicators. This study takes into account five process performance assessment indicators, which are described below. Figure 5 shows the process performance assessment indicators evaluated.

- **Fuel Efficiency ($\eta_{fuel}$):** the fuel efficiency is described as the ratio of total useful energy outputs to fuel inputs. The smallest systems, which use only the highest quality steam, have a fuel efficiency rating of 50%, while systems with low-grade thermal requirements and/or supplemental firing rate over 90%.
- **Electrical efficiency ($\eta_{el}$):** the electrical efficiency of the cogeneration plant refers to how effectively the plant converts biomass energy into electrical energy. Auxiliary electric power represents the total power needed to operate the plant and must be subtracted from the gross electric power produced to determine the net electric power output, which is crucial for efficiency calculations. This efficiency is calculated by dividing the electrical energy output by the total energy input from biomass sources, encompassing both thermal and electrical energy produced.
- **Overall plant efficiency ($\eta_{sys}$):** it is a measure to how effectively a plant converts its input energy into useful output energy. It considers all forms of energy inputs, such as sugarcane bagasse and straw and all useful outputs (gasoline, diesel and electricity). This indicator provides a comprehensive view of the plant's performance by accounting for both the primary product and any co-products or by-products. It is typically expressed as a percentage and calculated by dividing the total useful energy output by the total energy input.

Table 4 – Power generation and use in the biorefinery.

| **Power consumption** | **Electricity consumption (MW)** |
|---|---|
| Biomass grinding, transportation and feeding into the gasifier | 5.89 |
| Lean amine solution pump | 2.28 |
| Syngas booster compressor | 3.18 |
| PSA compressor | 0.36 |
| FT synthesis compressor | 0.96 |
| Hydroprocessing section unit | 5.72 |
| ASU compressor | 9.26 |
| Air Separation unit section | 20.83 |
| Sour gas shift steam compressor | 0.33 |
| $CO_2$ compressor | 1.29 |
| **Total power consumption** | **50.10** |
| **Power generation** | **Electricity generation (MW)** |
| Gas turbine | 69.50 |
| Steam turbine | 34.40 |
| **Total power generation** | **103.90** |
| **Net power exported to the grid** | **53.80** |

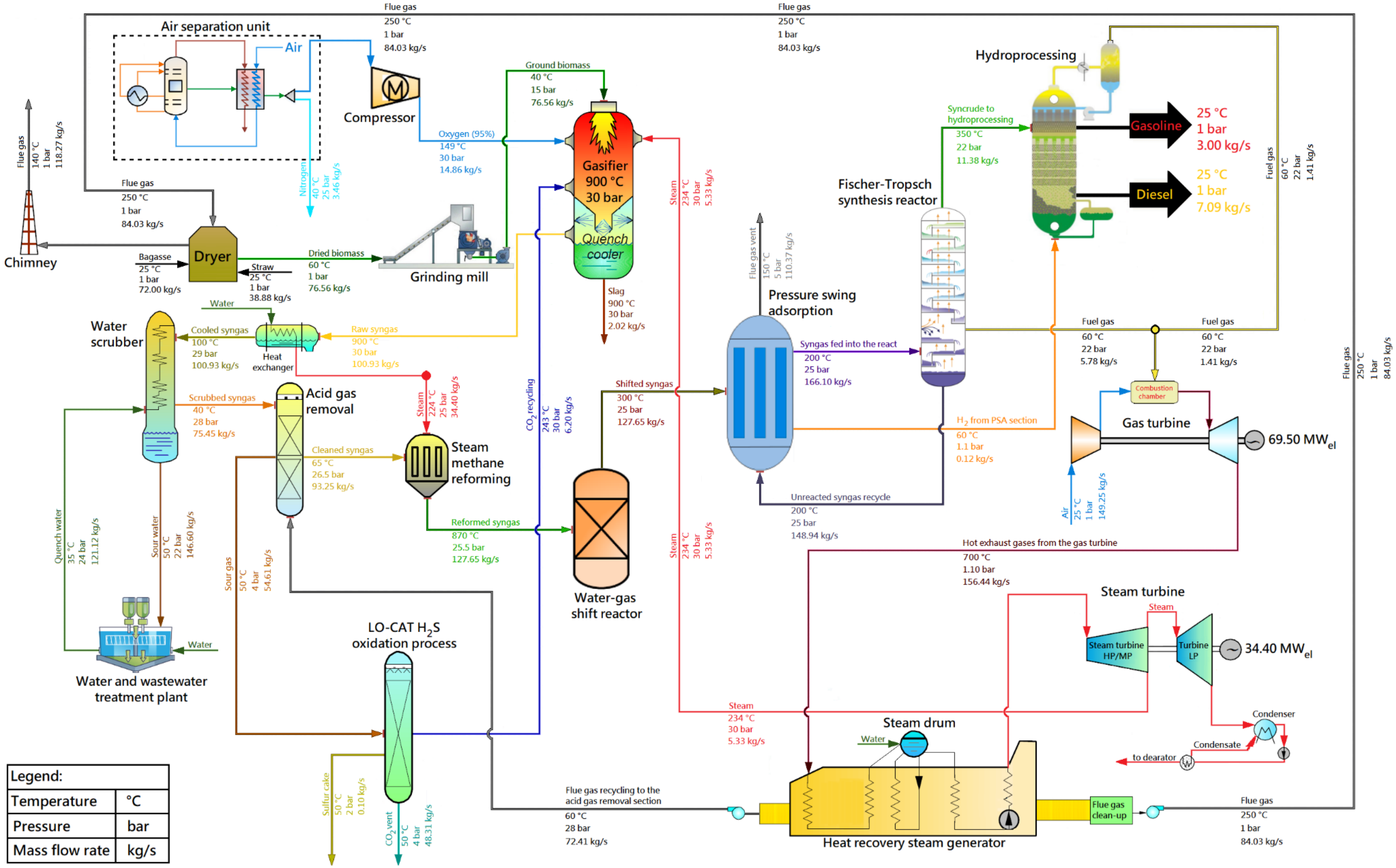



Figure 4 – Schematic of the biomass gasification configuration for the production of gasoline and diesel through FT synthesis and power generation evaluated in this work.

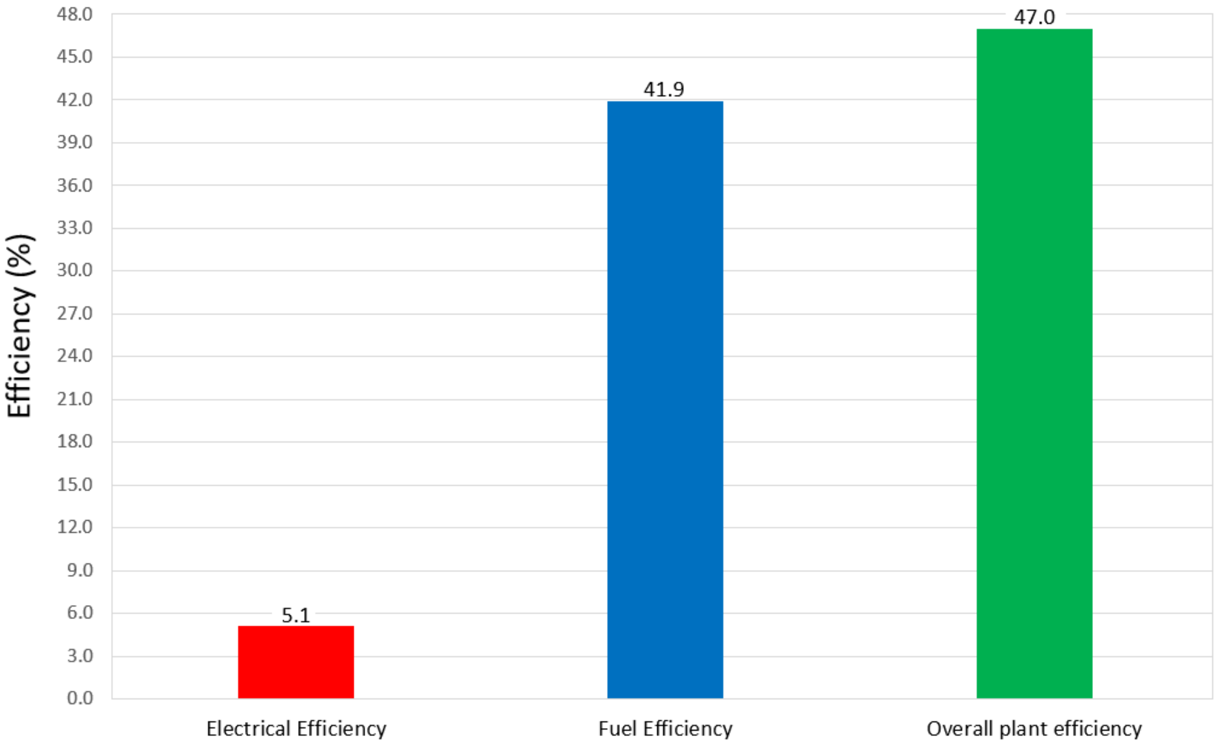


Figure 5 – Process performance assessment indicators.

## 4) Conclusions

This study presented a thermodynamic assessment of gasoline and diesel production through biomass gasification in the Brazilian sugarcane industry. The process involved several stages, from biomass pre-treatment to fuel synthesis and upgrading, utilizing Aspen Plus™ software for process modeling and simulation. One case scenario was evaluated, considering a total biomass flow rate of 110.8 kg/s. The developed gasification model considered the minimization of Gibbs free energy to determine the product composition, assuming isothermal and steady-state conditions. The synthesis of high-quality liquid fuels, such as gasoline and diesel, was achieved through biomass gasification, followed by raw syngas cleaning and syngas conditioning. The results showed that liquid fuel production is a viable and promising alternative, with an overall energy efficiency of 47%. The study demonstrated that integrating biomass gasification processes into sugar and ethanol plants can be a promising technological route for the production of renewable fuels, offering technical, environmental, and economic advantages.

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