UNIVERSIDADE ESTADUAL DE CAMPINAS
Faculdade de Engenharia de Alimentos

HENRIQUE REAL GUIMARÃES

AVALIAÇÃO TÉCNICO ECONÔMICA E AMBIENTAL DE ROTAS TERMOQUÍMICAS INTEGRADAS AO SETOR SUCROENERGÉTICO BRASILEIRO CONSIDERANDO ASPECTOS LOGÍSTICOS: VALORIZAÇÃO DESCENTRALIZADA DE BIOMASSA PARA COMBUSTÍVEL SUSTENTÁVEL DE AVIAÇÃO

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The most important words a man can say are, “I will do better.” These are not the most important words any man can say. I am a man, and they are what I needed to say.

The ancient code (...) says “journey before destination.” Some may call it a simple platitude, but it is far more. A journey will have pain and failure. It is not only the steps forward that we must accept. It is the stumbles. The trials. The knowledge that we will fail. That we will hurt those around us.

But if we stop, if we accept the person we are when we fall, the journey ends. That failure becomes our destination.

To love the journey is to accept no such end. ***I have found, through painful experience, that the most important step a person can take is always the next one.***

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RESUMO

O atual cenário de emissões crescente de GEE e os mais recentes relatórios acerca dos efeitos do aquecimento global criam um cenário preocupante. Esta situação clama por uma mudança na forma que a energia é produzida, distribuída e consumida. Em casos como a gasolina e diesel fóssil, já contamos com alternativas limpas e renováveis (bioetanol e biodiesel, respectivamente). Entretanto, para que consigamos atender as demandas de mitigação de carbono, outros setores devem aderir a essa mudança. Este é o caso específico do setor de aviação. Uma das rotas disponíveis mais aceita é a produção de combustível renovável de aviação (SAF) através da gaseificação de materiais lignocelulósicos seguido de Síntese Fischer-Tropsch para produção de combustíveis – a chamada rota GFT. Dada essa opção, o presente estudo avaliou diferentes aspectos relacionados à implementação desta rota junto ao cenário brasileiro. Através de análises técnico-econômicas assistidas por simulações (utilizando uma ferramenta computacional denominada Biorrefinaria Virtual), juntamente com uma revisão bibliográfica, essa tese estudou diferentes cenários implementando a rota GFT no Brasil, focando no uso de resíduos de cana (bagaço e palha) como principal matéria-prima.

A primeira etapa desse trabalho focou em avaliar os principais entraves à implantação da rota GFT, e em como o Brasil possui características vantajosas para viabilizar esse processo. Estudamos em detalhe os principais gargalos, tais como alto custo de investimento, baixa eficiência e altos custos de matéria prima. Através de um estudo de caso, comprovamos os benefícios de se integrar a rota GFT junta a usinas sucroenergéticas brasileiras. Dado condições convencionais de mercado, uma planta integrada GFT/usina 1G é capaz de atingir retornos próximos do desejado (taxas internas de retorno de 10 a 12% ao ano). Esses resultados foram expandidos ao se comparar o comportamento de uma planta standalone GFT com o cenário integrado. Estes resultados comprovaram que a integração é capaz de dobrar o retorno financeiro do processo, ao mesmo tempo que aumenta também as emissões evitadas de GEE.

Com o objetivo de avaliar outros aspectos que podem aumentar a viabilidade da planta GFT, este estudo também considerou mudanças da configuração logística. A descentralização da cadeia produtiva foi avaliada através do uso de unidades de Pirólise Rápida, densificando a biomassa em bio-óleo. Esta estratégia visou diminuir possíveis custos e impactos do transporte de matéria-prima até as unidades produtoras de SAF. Entretanto, esta configuração apenas se mostrou melhor que a opção centralizada para distâncias maiores que 1000 km entre o campo e a planta de GFT, devido aos custos para se produzir bio-óleo (que são de 2 a 5 vezes maiores que o custo de se produzir biomassa).

Uma das conclusões mais importantes desta tese é que, mesmo que nem todos os cenários propostos sejam economicamente viáveis, todos apresentaram bons resultados ambientais. Todos os cenários propostos são capazes de atender as demandas de mitigação de GEE com a substituição do querosene fóssil de aviação. Com o uso de politicas e incentivos governamentais, a mitigação de carbono pode ser convertida em receita adicional a fim de incentivar a produção e comercialização de SAF. Este tipo de prática seria capaz de favorecer o desenvolvimento da produção de renováveis e permitir atingir as metas propostas nos diversos acordos e mandatos de redução de emissões.

ABSTRACT

The current scenario of growing GHG emissions and the latest reports on the global warming trends paint a worrisome picture. This urges for changes on the way energy is produced, distributed and consumed. Some renewable and clean alternatives already exists, such as bioethanol and biodiesel as substitutes for fossil gasoline and diesel, respectively. However, in order to achieve the goals for carbon mitigation by 2050, other sector must also suffer changes, particularly the aviation sector. One of the most accepted alternatives for the aviation sector is the production of sustainable aviation fuel (SAF) through the gasification of lignocellulosic biomass, followed by catalytic conversion (Fischer-Tropsch reactions), the so-called GFT route. With this option in mind, the present study evaluated different aspects of implementing this route into the Brazilian market. By carrying out a techno-economic analysis aided by a simulation framework (the Virtual Biorefinery), alongside a thorough bibliographic review, the present thesis managed to study different scenarios and options for implementing the production of SAF in Brazil using the GFT route.

The first stage of this project focused on evaluating the main setbacks of the GFT route, and how the Brazilian bioenergy infrastructure could be a viable option for implementing this process. We studied in detail the most important bottlenecks such as the high equipment costs, low industrial process efficiency, and high feedstock prices. Through an initial case study, we managed to demonstrate the benefits of integrating the GFT route into the existing 1G ethanol biorefinery structure. Under normal market conditions, a greenfield GFT/1G mill integrated plant would be very close to the range of economic viability (IRR from 10-12% per year).

These results were expanded and validated by comparing the economic and environmental performance of a standalone GFT plant to a scenario where this unit is integrated into a sugarcane mill/ethanol distillery. The results showed that the integration was able to improve the economic performance of the BtL route, almost doubling the internal rate of return of the plant. The environmental performance of the plant also benefits from the integration, increasing the total avoided GHG emissions compared to the standalone BtL plant.

Aiming to evaluate other aspects that may improve the viability of BtL plants, changes to the logistic chain configuration were also considered. We evaluated the decentralization of the production chain with the use of fast pyrolysis (FP) units to densify the biomass into bio-oil. This strategy aimed to reduce feedstock transportation costs. This option, however, was only more viable than a centralized production for distances greater than 1000 km between the biomass production sites and the SAF production units. The cost of producing bio-oil is 2 to 5 times higher than using the biomass directly on the GFT process.

One of the most important conclusion of the present study is that even though some of the proposed routes are not economically attractive, all of them presented good environmental results. All the proposed scenarios were able to meet the demands for GHG mitigation by substituting fossil aviation fuel in the Brazilian market. With the use of governmental policies and subsidies, such as the RENOVABIO, this carbon mitigation could be converted into additional revenue to incentivize the production and commercialization of SAF, and help achieving the goals of the different agreements and GHG mitigation mandates.

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ABREVIATIONS

1G – First generation

2G – Second generation

BtL – Biomass-to-Liquids

CAPEX – Capital expenditure

CBio – Decarbonization credits

CNPEM - Brazilian Center for Research in Energy and Materials

$CO_{2\ eq}$ – Equivalent carbon dioxide emission

d.b. – Dry basis

FT – Fischer-Tropsch synthesis

FP – Fast pyrolysis

GFT – Gasification/Fischer-Tropsch synthesis

GHG – Greenhouse gases

GWP – Global warming potential

IEA – International Energy Agency

IPCC - Intergovernmental Panel on Climate Change

IRR – Internal rate of return

INT – Integrated configuration

LCA – Life cycle assessment

LCM – Lignocellulosic material

LNBR – Brazilian Biorenewables National Laboratory

NPV – Net present value

O&M – operation and maintenance

OPEX – Operational expenditure

RENOVABIO – National Biofuels Policy

SA – Standalone configuration

SAF – Sustainable aviation fuels

VB – Virtual Biorefinery

w.b. – wet basis

SUMMARY

Chapter I - Introduction

Much has changed in the past five years since the present project started. Initially, the motivation was to develop new ways to produce energy in a clean and environmental-friendly way. International agreements for GHG emissions mitigation, such as the COP 21 (FEDERATIVE REPUBLIC OF BRAZIL, 2022) have created the need to study and evaluate new alternatives for the current status-quo of energy production and consumption. This is even more necessary for sectors without long-term solutions for biofuels, such as the aviation sector (IRENA, 2017) with the demands from the CORSIA mechanism (SOARES and CENAMO, 2018).

However, for the past couple of years the world has found itself amidst a global economic crisis aggravated by a worldwide pandemic outbreak. Despite the temporary decrease in the energy consumption due to the COVID, the global emissions of GHG into the atmosphere kept rising, and the period between 2015-2021 were the warmest seven years in recorded history IEA, 2021).

The escalation of GHG emission in the current scenario intensifies the urgency of increasing the efforts to find better alternatives. The most recent reports by IEA (IEA, 2017 and 2021) and IPCC (IPCC, 2014) point out the need to quickly change the mindset and improve the uptake of clean energy in different sectors. Indeed, according to IEA over half of the necessary GHG reductions will come from technologies that are still at the demonstration or prototype stage, thus indicating that the efforts in research is needed more now than ever.

Such a scenario is the case for the aviation sector, where demand for liquid fuels is expected to grow steadily (MCKINSEY, 2022), despite a lack of available fuel options to achieve carbon neutrality by 2050 (IEA, 2021). Besides that, international agreements like the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) aim to force the mitigation of emissions on the sector. Not only that, but mechanism such as the ReFuelEU aims to enforce fuel suppliers to distribute clean fuels at European Union airports (SOONE, 2022).

Four routes approved by the ASTM can supply the demand of sustainable aviation fuel. The Synthesized Iso-Paraffinic (SIP) route can produce fuels directly from sugars, and the Alcohol-to-Jet (ATJ) process is based on converting alcohols (mainly isobutanol) into jet fuel. The Hydroprocessing of Esters and Fatty Acids (HEFA) is currently the most mature route.

However, feedstock costs and sustainability concerns make it difficult to ramp up production to meet rising demand. (IRENA, 2017). The route comprised of Gasification of biomasses followed by Fischer-Tropsch synthesis (GFT process) comes as a viable option to help supply this demand. This route is able to process low-grade feedstock (CORMOS et al., 2015) into a large array of products such as advanced biofuels with similar characteristics to conventional fossil fuels, with the advantage of near-zero sulfur content and low pollutants emission (BALIBAN et al., 2013; TRIVEDI et al., 2015; RAFATI et al., 2017; KLEIN et al., 2018).

Even though the GFT technology has been used since the 1940s to convert fossil sources into liquid fuels (VAN VLIET et al., 2009; HAARLEMMER et al., 2012), biomass gasification plants have yet to demonstrate large-scale industrial success (RAFATI et al., 2017) due to some barriers mainly associated with technological and logistical aspects. High equipment costs (TAN et al., 2016; DIMITRIOU et al., 2018) and the challenges to adapt the technology for biomass conversion (MOTTA et al., 2018) are the main problems this route faces. One possible strategy to help make it feasible for biomass conversion is the integration of the GFT route with other well-stablished industrial processes. This option promotes technological synergies and expand the product portfolio (PETERSEN et al., 2015; DIEDERICHS et al., 2016; ALVES et al., 2017; KLEIN et al., 2018; BRESSANIN et al., 2020), helping alleviate production costs by distributing the expenses among other by-products. Other possible solution is to stablish long-term biomass supply chain (ALVES et al., 2017; DIMITRIOU et al., 2018).

Both the approaches of integration and supply chain optimization have the potential to increase the economic performance of the GFT route, and the Brazilian bioenergy sector is a promising scenario to evaluate the implementation of such route. The country presents a well-developed supply chain of different biomass sources. An estimation presented by the RSB-Roundtable on Sustainable Biomaterials (2021) indicates that over 30 Mtonnes of sugarcane bagasse, 20 Mtonnes of sugarcane straw, and over 20 Mtonnes of eucalyptus residue are available around to country to produce SAF. This availability highlights the potential of using this existing infrastructure to help implement the GFT route.

The country already counts with an existing infrastructure and a well-established bioenergy production chain in the form of the sugarcane industry, capable of producing over 33 billion liters of biofuel with the added bonus of a large production of lignocellulosic residues available for further valorization (SUCRE, 2017; CONAB, 2019; LEAL and HERNANDES, 2020; UNICADATA, 2020). This scenario act as a suitable base for the implementation of new biofuels production routes thanks to the existing expertise and the available supply chain of biomass. The country has also recently created a carbon credits market to incentivize fuel producers and distributors to adhere to the use of biofuels (DE SOUZA, et al., 2018). Some studies already indicate the benefits of integrating the GFT process into the first generation (1G) ethanol production (KLEIN et al., 2018; BRESSANIN et al., 2020).

In order to overcome the technical and economic challenges, it is assumed that the economy of scale is necessary to make the biomass gasification process feasible (WRIGHT et al., 2008; ERANKI and DALE, 2011; LI et al., 2015; DIMITRIOU et al., 2018). As this implies the need to process large amounts of biomass in a single industrial plant (WRIGHT and BROWN, 2007), attention should be given to the logistical aspects of feedstock transportation. One interesting option is to make use of the diverse biomass supply and build a distributed production chain with densification units in order to diminish costs with feedstock and to be able to benefit from economy of scale (WRIGHT et al., 2008, YOU and WANG, 2011; ZHENG et al., 2016).

The process of fast pyrolysis can act as a densifying unit for the GFT route, acting as smaller scale biomass “pretreatment” stage, improving the feedstock physical properties and fuel quality. Fast pyrolysis consists on the use of moderate temperatures (around 500 °C) with absence of oxygen, first with the evaporation of water from the biomass followed by decomposition and volatilization of its components. The main product is the so-called bio-oil, a complex mixture of phenolic compounds, organic acids, hydrocarbons and other chemicals. Due to its varied composition, bio-oil can be used to for energy generation (BRIDGWATER, 2012), upgraded to produce an array of fuels and chemicals (LI et al., 2015), and may be an ideal material for gasification (ZHENG et al., 2016). Since some studies point that, compared to gasification units, pyrolysis units are less dependent on scale to be economically viable (WRIGHT and BROWN, 2007), and considering the high density of bio-oil, this product may prove itself as an important asset to the production chain. This could lead to lower transportation costs compared to raw biomass, thus resulting in larger optimally sized fuel production facilities and lower unit costs for fuel (WRIGHT et al., 2011; VAN DER STELT et al., 2011).

With these considerations, this thesis proposes to study different scenarios integrating the GFT route to the Brazilian sugar-energy sector, evaluating the entire production chain for each of them in terms of its economic performance and environmental impact. These analyses should account for the configuration of the GFT route, the integration with the 1G ethanol production chain, the commercialization of carbon credits based on the avoided carbon emissions, and finally the assessment of using fast pyrolysis units to decentralize the production chain as a mean to lower SAF production costs.

On a broader context, the present project was developed alongside the PITE/FAPESP project entitled “Whole chain decentralized biomass valorization to advanced biofuels: development and assessment of thermochemical routes integrated to biomass production and biochemical routes – H2020 BioValue”. This larger project involves different research facilities, universities and companies, and focuses on the study of different routes for the production of advanced biofuels. Among the proposed analysis, the production of SAF through the GFT route is the main option, including the study of decentralization options. Thus, the present thesis was made as a basis for the development of the BioValue project.

Chapter II - Objectives

The main hypothesis of the proposed project is that the process of gasification/Fischer-Tropsch conversion has the potential to be a suitable mean to produce sustainable aviation fuel on a scenario integrated into the Brazilian sugarcane sector, and the development of a decentralized production chain could benefit the viability of this process.

The overall objective of the present project is to assist the decision-making process seeking for viable routes to obtain advanced fuels, with focus on thermochemical technologies and assessing the possible tradeoffs between economic and environmental impacts. This evaluation centers around the large-scale production of renewable biojet fuel through gasification and Fischer-Tropsch conversion routes integrated to the Brazilian sugarcane sector.

The main original contribution of this work is to consider the integration between these different routes and evaluate the influence of the addition of smaller scale densifying units based on the concept of bio-oil production from fast pyrolysis, receiving sugarcane biomass residues (bagasse and straw from biochemical routes at sugarcane mills) and supplying bio-oil to a central gasification unit.

The specific objectives of the project can be divided into four main steps. The first stage is the selection of the feedstock supplying scenario, and the choice between centralized or decentralized production chain.

The second specific objective is the detailing of the conversion route, both for the decentralized units, and the fuel synthesis units (gasification and FT synthesis). This alternative is defined by the selection of the desired set of processes (biomass gasification followed by FT technology; or biomass pyrolysis followed by bio-oil gasification and FT conversion), and the plant configuration (standalone or integrated).

The process simulation is the focus of the third specific objective, which is a crucial part of the proposed work. The emphasis is on the design of the route to provide the means to calculate the mass and energy balances of the processes, the consumption of feedstock/other inputs and the generation of products and byproducts. This step consists on the collection of data based on the scenarios defined in the previous 2 steps. The agricultural stage and the 1G industrial stage data are available from the Virtual Biorefinery. The bulk of the effort in this project was dedicated to the modelling and simulation of the thermochemical processes such as gasification, Fischer-Tropsch conversion and fast pyrolysis.

The fourth objective focus on the evaluation of the scenarios. This includes techno-economic analysis and life cycle assessment. Both the economic and environmental indicators in this thesis take into account logistics aspects when considering the influence of the industrial scale and the dependence on large amounts of biomass, focusing on the feedstock (transportation, distances, type of transportation) and bio-oil (stabilization costs, transportation, storage, distances and type of transportation). These analyses also include the uncertainty assessment of each evaluated output, to determine the influence of the different parameters and test the robustness of our models.

Chapter III - Review Article

The following paper was accepted and published in Energy Conversion and Management, vol. 245 on August 16th, 2021. The scope of this work was to provide a review of the current scenario of BtL routes, the main challenges for its application and the most viable strategies and solutions for improving the process economic feasibility. The paper also provides a case study to show the potential of implementing the GFT route integrated into the Brazilian sugarcane sector.

Bottlenecks and potentials for the gasification of lignocellulosic biomasses and Fischer-Tropsch synthesis: A case study on the production of advanced liquid biofuels in Brazil

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Abstract

Brazil is one of the major players in the biofuels market worldwide, and its existing biorefining infrastructure can be used as the basis to support the implementation of new advanced biofuel production routes at a large scale. This paper demonstrates the benefits of the integration of both biochemical and thermochemical processes and how this configuration has the potential to overcome the main barriers that the Biomass-to-Liquids (BtL) route currently faces. Important bottlenecks such as the high equipment costs, low industrial process efficiency, and high feedstock prices were studied in detail by assessing a series of production scenarios that take into account the Brazilian context for building new biorefinery plants. By carrying out a techno-economic analysis aided by a simulation framework (the Virtual Sugarcane Biorefinery), we evaluated the potential technological synergies of a BtL plant processing sugarcane bagasse and straw integrated into a first-generation sugarcane ethanol distillery. Results in this paper indicate that it is possible to achieve economic feasibility with the implementation of the BtL route in the country. Under a base scenario, a greenfield plant would be very close to the range of economic viability (IRR from 10-12% per year), whereas more optimistic economic conditions (e.g., lower CAPEX and higher fuel prices) would induce even better results (IRR >16% per year). Doubling the milling capacity also favors the BtL process, with IRR reaching 20% per year if the best economic conditions are achieved in the Brazilian context.

Keywords:

Biojet fuel; sugarcane; techno-economic analysis; thermochemical conversion; gasification; Fischer-Tropsch

Highlights:

1. Existing sugarcane biorefineries in Brazil are the main advantage to implement BtL route;
2. High costs of equipment and technologies are the main challenges to economic viability;
3. Bioethanol commercialization helps to make the integrated BtL plant feasible;
4. Base case presents IRR close to the minimum rate accepted by the sector (10-12%);
5. Lower equipment costs and higher ethanol prices combined to improve the process viability

1 - Introduction

With the worldwide interest in alternative energy sources as a solution to mitigate the effects of climate change, large-scale renewable fuel use is a reality in some regions of the world aiming to reduce greenhouse gas (GHG) emissions. In Brazil, particularly, biofuels have been extensively produced since the 1970s, contributing to an energy matrix with almost 50% of renewable energy sources [1]. Besides this historical learning curve of developing and implementing bioenergy solutions, an additional push towards bioenergy is introduced with the different international agreements and commitments for carbon emissions and green policies. The country committed to a Nationally Determined Contribution to reduce GHG emissions by 37% by 2025 compared to 2005 levels [2] and implemented the National Biofuels Policy (RenovaBio) to establish decarbonization goals for the fuels sector, with the creation and commercialization of carbon credits to encourage fuel producers and distributors to adhere to this policy [3,4].

These mechanisms are in motion and are supported by the established biofuel production infrastructure (bioethanol as a substitute for gasoline, and biodiesel for fossil diesel). Therefore, particular interest lies in finding solutions for the demands of fuels without a consolidated long-term biofuel alternative such as long-haul transportation fuels. This is the case of aviation fuels since Brazil and many other countries are committed to the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA), which would imply a reduction of at least 1.5 million tonnes of CO_2 in the aviation sector just to achieve the minimum requirements by 2030 [5].

Currently, the Hydroprocessing of Esters and Fatty Acids (HEFA) is the most mature route for biojet fuel production from biomasses [6,7]. However, the costs associated with oleochemical feedstocks are elevated, and their use implies supply and sustainability/environmental concerns, which make the scale-up of the HEFA process difficult to meet the market demands [6,7]. Moreover, according to IRENA [6], more than 400 Mtonnes of biojet fuel would be required by 2050, and HEFA cannot supply it entirely, as its current production capacity corresponds to less than 1.5% of the global jet fuel demand [8]. Besides, the same raw material is used for biodiesel production, making it even more difficult to increase jet fuel production with this route. Therefore, the supply chain of other sustainable alternatives is still under development.

Among the available routes to supply the global jet fuel demand, thermochemical processes are the most likely to be used [6]. The gasification followed by the Fischer-Tropsch (FT) synthesis (GFT process) has been used since around 1940 to process coal into liquid fuels (Coal-to-Liquids – CtL) [9], and can also process low-grade feedstock [10] into a large array of hydrocarbons and phenolic compounds, which includes advanced biofuels (Biomass-to-Liquids process – BtL). As the BtL route produces green diesel and green gasoline besides biojet fuel, it does not compete with biodiesel production as in the case of the HEFA process. These biofuels have similar characteristics to conventional petroleum-derived transportation fuels and are compatible with the available infrastructure for fuel transportation and storage as well as vehicle engine designs, with the advantage of near-zero sulfur content and low pollutants emission [11] such as NO_x, particulates, aromatics, and CO. Overall, these routes can achieve GHG emissions 80% lower than those from fossil fuels [7,12,13].

Despite this promising environmental performance, the BtL technology is still at an early stage of implementation, and gasification plants are present only at a demonstration stage in terms of technology readiness level [14]. The main barriers for large-scale BtL applications are mainly associated with technological aspects, with the challenge of adapting the conversion technology to different types of biomass and also of improving the syngas cleaning process

[15]. Moreover, the high equipment costs [16,17] reduce the economic competitiveness of BtL biofuels since the current plant capacities for their production still fall short of exploring the full benefits of higher economies of scale. Motta et al. [15] also raised the dependence of the BtL routes upon the biomass supply chain, in a way that an unstable or immature biomass market can hinder investments.

In the Brazilian case, the existing infrastructure and the expertise of its well-established bioenergy industry may act as a more favorable environment to develop new technological routes such as the thermochemical process. This is especially true for the sugarcane industry, with a strong presence in the country producing sugar, electricity, and over 33 billion liters of bioethanol during the 2018/2019 season [18]. This industry also produces large amounts of sugarcane bagasse, a lignocellulosic residue available for further valorization through the so-called second-generation (2G) fuel production routes. It is worthwhile mentioning that the sugarcane bagasse is already available at the production site avoiding logistic costs. In 2016, more than 178 million tonnes of bagasse were produced in the country [19]. Other than bagasse, sugarcane cultivation also produces large amounts of sugarcane straw that are usually left on the fields [20], while a large fraction of this material could be used for thermochemical conversion. According to the SUCRE project [20,21], more than 40 million tonnes of sugarcane straw (dry basis) were produced during 2017.

The present study proposes an assessment of BtL plants in Brazil for biofuels production, highlighting the potentials and setbacks, as well as assessing strategies to implement this route according to the specificities of the Brazilian context, which may favor the large-scale development of the BtL technology sustainably. To illustrate that and to indicate favorable scenarios for the implementation of Gasification and FT technologies, a case study was elaborated considering these guidelines into a Brazilian biorefinery concept. The scenarios were implemented based on solutions raised in European and North-American contexts that may be applicable for the Brazilian scenario, such as the integration of BtL plants into an existing biofuel production chain. Therefore, this work considered the integration of a BtL plant into a first-generation (1G) sugarcane ethanol distillery, where the residues (bagasse from the process and straw from the fields) are used as feedstock for a BtL plant that produces biojet fuel.

2 - Economic feasibility: main bottlenecks

Although many studies have assessed the environmental impacts of BtL routes [7,12,13,22–24], few studies have focused on the large-scale deployment of this technology in commercial plants. While fossil feedstock-based GFT plants have been in operation around the globe since the 1940s and some are still under operation [9,25], BtL plants, however, have yet to encounter an industrial application, with mainly pilot and demonstration facilities being developed [11]. Table III-1 presents an overview of the BtL plants worldwide that rely on biomass gasification followed by FT conversion. As is evident, the majority of these plants are pilot scale, with most of the commercial plants either canceled or under planning/construction. The number of canceled BtL plants is a concern, and it might be a reflection of the bottlenecks found in biomass gasification and syngas processing technologies [26–28], in a way that some technological and economic barriers still need to be overcome.

Table III-1 – Lignocellulosic biomasses BtL plants. Source: [29]

Plant	**Owner**	**Status**	**Country**	**Scale**	**Liquid fuels yearly production**	**Biomass**
Choren beta plant	CHOREN Industries GmbH	Canceled	Germany	Commercial demo*	13,500 t	Forest residues
Choren sigma plant	CHOREN Industries GmbH	Canceled	Germany	Commercial demo	200,000 t	Forest residues
Genesis	Cool Planet	Canceled	USA	Commercial demo	30,000 t	Forest residues
Trixie	Flambeau River Biofuels Inc.	Canceled	USA	Commercial demo	51,000 t	Forest residues
Choren alpha plant	CHOREN Industries GmbH	Idle	Germany	Pilot	53 t	Wood and forest residues
BIOENERGY 2020+	Vienna University of Technology / BIOENERGY 2020+	On hold	Austria	Pilot	1.5 t	Lignocellulosic biomass
BioTfuel	BioTfuel	Operational	France	Pilot	60 t	Forest waste, straw, green waste, dedicated crops
Synthesis Cutec Clausthal-Zellerfeld	Cutec	Operational	Germany	Pilot	0.02 t	Straw, wood, dried silage, organic residues
Des Plaines plant (GTI gasifier)	Gas Technology Institute (GTI)	Operational	USA	Pilot	38 m^3	Pellets, wood chips
Southern Research Institute Pilot Plant	Southern Research Institute	Operational	USA	Pilot	0.002 t	Cellulosics, Municipal wastes
TRIJEN	TUBITAK	Operational	Turkey	Pilot	250 t	Hazelnut shell, olive cake, wood chip, and lignite blends
Red Rock Biofuels	Velocys	Under construction	USA	Commercial demo	44,000 t	Forest residues

demo: demonstration

One of the factors that prevent the scale-up of BtL plants is their economic viability. Table III-2 presents a collection of works that investigated the techno-economic aspects of BtL plants from 2011 to 2017. Overall, most of the studies indicate that biofuels produced through gasification and FT synthesis are not competitive with fossil fuels yet. For example, Hunpynio et al. [30] observed that the integration of the BtL process with a gasification plant for power generation in Thailand would produce green diesel for a cost more than 40% higher than that obtained from fossil sources. The authors observed lower investment risks in the case of very high fossil fuel prices. Diederichs et al. [31] investigated the production of biojet fuel through different processes, namely gasification and FT synthesis, biochemical conversion to ethanol with upgrading, gasification followed by syngas fermentation to ethanol with upgrading, hydroprocessing of vegetable oil, and fermentation of sugarcane juice to ethanol with upgrading. The authors verified that neither of these routes could achieve a minimum fuel selling price lower than that the fossil-based jet fuel price (0.42-1.28 US$/kg).

However, some studies indicate a more favorable scenario. Jiang and Bhattacharyya [32] reported viable results of green gasoline and diesel production through biomass gasification and FT synthesis under certain scenarios of higher oil prices and plants with higher capacities. Nevertheless, when considering lower crude oil prices (around 60 U$/barrel), almost none of the studied designs would be feasible, except for larger-scale plants (50,000 barrels per day) coprocessing coal and biomass, showing a decrease of about 57% on their current costs.

Table III-2 - Survey of techno-economic results for BtL route studies

Feedstock	**Site**	**Configuration**			**Products**		**Economic result**			**Ref**
		Value	**Unit**	**Integration**	**Fuels**	**Other**	**Value**	**Index**	**Base Year**	
Generic BM										
Generic BM	USA	614	ktonne/year (dry BM)	-	**JF**, N	Electricity	244.2	MSP (¢/kg)	2014	[31]
Generic BM	NO	19.2	tonne/h (fuels)	BtL	**D**, JF, N, LPG	Heat, residues	2.36	PC ($/L)	2017	[33]
		46	tonne/h (fuels)	PBtL	**D**, JF, N, LPG	Heat, residues	1.74	PC ($/L)	2017	
Generic BM	DE	90	ktonne/year (fuels)	Pyrolysis	JF	-	2.43	PC (€/kg)	2014	[34]
				Pyrolysis + PBtL	JF	-	3.07	PC (€/kg)	2014	
Woody BM										
Hardwood	USA	264	kB/year	-	JF, G, D	-	23.25	PC ($/GJ)	2011	[12]
		330	kB/year	-	JF, G, D	-	21.71	PC ($/GJ)	2011	
		825	kB/year	-	JF, G, D	-	17.9	PC ($/GJ)	2011	
		3,300	kB/year	-	JF, G, D	-	14.13	PC ($/GJ)	2011	
Wood chips	TH	200	tonne/year (fuels)	Power generation	D	Electricity	-0.2	RoI (%)	2013	[30]
		450	tonne/year (fuels)	Power generation	D	Electricity	0.6	RoI (%)	2013	
		750	tonne/year (fuels)	Power generation	D	Electricity	0.8	RoI (%)	2013	
Wood chips	SE	430	MW (LHV BM)	-	D, G	Electricity	84-125	PC (€/MWh)	2012	[35]
				CCS	D, G	Electricity	94-107	PC (€/MWh)	2012	
				Oil refinery	D, G	Electricity	74-109	PC (€/MWh)	2012	
				Oil refinery + CCS	D, G	Electricity	82-92	PC (€/MWh)	2012	
Coal and wood chips	USA	3,333	kB/year	CCS	D, G	-	11.5	IRR (%)	2013	[32]

		10,000	kB/year	CCS	D, G	-	12.2	IRR (%)	2013	
		16,667	kB/year	CCS	D, G	-	14	IRR (%)	2013	
		3,333	kB/year	-	D, G	-	12	IRR (%)	2013	
		3,333	kB/year	CCS	D, G	(low oil price)	6.1	IRR (%)	2013	
		16,667	kB/year	CCS	D, G	(low oil price)	8.5	IRR (%)	2013	
Eucalyptus residue	BR	102	ktonne/year (JF)	-	JF, N, D, LPG	Biochem.	4-9.3	IRR (%)	2014	[36]
Pinus residue				-	JF, N, D, LPG	Biochem.	0-6.6	IRR (%)	2014	
Wood	EU	136	Mtonne/year	-	JF, G, D	-	18.46	PC (€/GJ)	2014	[16]
		143	Mtonne/year	-	JF, G, D	-	17.88	PC (€/GJ)	2014	
Wood	NO	60-239	Ml/year (BC)	Torrefaction;CCS	BC	-	14-34	PC ($/GJ)	2014	[37]
Willow	DE	800	ktonne/year (fuels)	Torrefaction	D, N, JF	-	1054	PC (€/tonne)	2014	[24]
Sawdust	USA	400	MW (LHV BM)	-	FT liquids	-	~30	PC (€/GJ)	2015	[11]
				-	FT liquids	Electricity	~36-43	PC (€/GJ)	2015	
Sawdust + natural gas	USA	400	MW (LHV BM)	-	FT liquids	-	~20-22	PC (€/GJ)	2105	
Residues and crops										
Corn stover	USA	5	kB/day	-	JF, D	-	1.46-2.54	SC ($/gal)	2012	[13]
Corn stover	USA	75.3	ktonne/year (JF)	-	D, N, JF	Electricity	~10	IRR (%)	2015	[38]
Rice residues	BR	102	ktonne/year (JF)	-	JF, N, D, LPG	Biochem.	1.7-7.7	IRR (%)	2014	[36]
Coffee residues	BR	102	ktonne/year (JF)	-	JF, N, D, LPG	Biochem.	0-6.7	IRR (%)	2014	

Sweet sorghum	BR	102	ktonne/year (JF)	Annexed (1G + 2G)	JF, N, D, LPG	Biochem.	0-5.9	IRR (%)	2014	
Sweet sorghum residues	BR	102	ktonne/year (JF)	-	JF, N, D, LPG	Biochem.	0-6.1	IRR (%)	2014	
Wheat straw	DE	800	ktonne/year (fuels)	Pyrolysis	D, N, JF	-	1680	PC (€/tonne)	2014	[24]
Sugarcane bagasse	ZA	6,500	l products/h	Sugarcane mill	D, N	Electricity	9.7	IRR (%)	2012	[39]
		9,433	l products/h	Sugarcane mill	D, N	Electricity	16.9	IRR (%)	2012	
Sugarcane	BR	102	ktonne/year (JF)	Annexed (1G + 2G)	JF, N, D, LPG	Biochem.	0.4-7.8	IRR (%)	2014	[36]
Sugarcane residues	BR	102	ktonne/year (JF)	-	JF, N, D, LPG	Biochem.	0-8.6	IRR (%)	2014	
Sugarcane bagasse	USA	116	ktonne/year (JF)	-	D, N, JF	Electricity	~12	IRR (%)	2014	[38]
Sugarcane	BR	4	Mtonne/year (BM)	Sugarcane mill	JF, D, N, EtOH	Electricity	16.5	IRR (%)	2015	[7]
Sugarcane, eucalyptus	BR	4	Mtonne/year (BM)	Sugarcane mill	JF, D, N, EtOH	Electricity	13.5	IRR (%)	2015	
Coal and bagasse	USA	3,333	kB/year	CCS	D, G	-	11.4	IRR (%)	2013	[32]
Sugarcane, eucalyptus	BR	4	Mtonne/year (BM)	Sugarcane mill	JF, D, N, EtOH	Electricity	9.4	IRR (%)	2017	[40]
Energy cane, eucalyptus	BR	4	Mtonne/year	Sugarcane mill	JF, D, N, EtOH	Electricity	6.2	IRR (%)	2017	
Fossil fuels										
					JF		42-128	MSP (¢/kg)	2014	[31]
							500	PC (€/tonne)	2017	[24]
					D		78-92	PC (€/MWh)	2012	[35]

		16.2	PC (€/GJ)	2014	[16]
	G	16.6	PC (€/GJ)	2014	

BC: biocrude; BM: biomass; BR: Brazil; BtL: biomass-to-liquids; CCS: carbon capture and storage; CO: crude oil; D: diesel; DE: Germany; EtOH: ethanol; EU: Europe; FT: Fischer-Tropsch; G: gasoline; IRR: Internal Rate of Return; JF: kerosene (jet fuel); kB: thousand barrels; LHV: lower heating value; LPG: liquefied petrol gas; MSP: minimum selling price; N: naphtha; NO: Norway; PBtL: power and biomass-to-liquids; PC: production cost; RoI: Return on Investment; SC: supply cost; SE: Sweden; TH: Thailand; USA: United States of America; ZA: South Africa

Oil prices play a major role in determining the feasibility of renewable fuel production routes. Pereira et al. [38] indicated that biofuels production is highly susceptible to competition with crude oil, and the price of this commodity is one of the main factors that determine the internal rate of return (IRR) of BtL plants. This dependency leads to scenarios of higher unpredictability due to crude oil price fluctuations [36]. The main contribution to the low competitiveness with crude oil lies with the relatively high production costs of the BtL route due to high capital investment, low fuel product output, and high biomass costs [16].

2.1.Investment costs and equipment manufacturing

Overall, the expenses associated with equipment and installation are the main contributors to the production costs. Different from other production pathways, where capital costs comprise less than 15% of the total supply costs, the share of equipment and installation costs for FT fuels are more expressive [13]. In many studies, the capital expenditure (CAPEX) contribution exceeds 30% of the fuel production costs and, consequently, is responsible for the largest share of the minimum selling price of BtL fuels [12,41].

This high capital investment is mainly due to the equipment and operations necessary for the gasification of the biomass and the ensuing syngas cleaning and conditioning [16,17]. To illustrate this, Baliban et al. [12] and Bressanin et al. [40] found that the investment necessary to produce clean syngas from lignocellulosic biomass may translate into almost half of the overall cost of the plant. Syngas cleaning needs to remove several undesired impurities from the gas (such as NH_3, H_2S, tar, HCl, and alkaline metals) and thus corresponds to a series of complex and potentially expensive group of industrial processes [15].

Another reason for the relatively high production costs of BtL fuels is that many of the required technologies and equipment are proprietary and must be imported in many cases. With the resulting location factors and the high exchange rate between currencies, these costs are further pronounced when the equipment is imported to developing countries [7].

The high installation costs can be somewhat reduced by relying on economies of scale. The increase in these costs caused by an expansion on capacity is not so pronounced relative to the gains in production, thus reducing the impact of the production costs and improving the economic performance of the processing route [12,30]. For example, Jiang and Bhattacharyya

[32] verified that the IRR of a coal and woodchip gasification/FT plant increased from around 11% up to 15% by increasing the capacity from 10,000 to 50,000 barrels per day. This result corroborates that plant size is a very important parameter affecting the competitiveness of thermochemical processes.

2.2.Fuel output

Another factor that adds up to high investment costs is the process energy efficiency. Rafati et al. [11] observed that around 40% of the biomass energy (on a lower heating value basis) is converted into FT liquids. Neuling and Kaltschmitt [24] found similar results with energy efficiencies ranging from 30 to 38%.

The low process efficiencies of BtL routes can be related to the mass yields, especially because FT reactions have low overall conversions [30]. While evaluating the carbon flow diagram of a BtL process, Dietrich et al. [34] highlighted that there is a high loss of carbon during the process in the form of CO_2 (around 70%) and, therefore, a significant fraction of the carbon present in the biomass is not converted into the final product. Normally, part of the biomass is converted into CO_2 during gasification and the adjustment of the H_2/CO ratio in the syngas stream via water-gas shift reaction is required. During this stage, part of the CO reacts with water to form more hydrogen and, therefore, part of the carbon is converted and inevitably released in the form of CO_2 [11]. According to Neuling and Kaltschmitt [24], the BtL process involves the destruction of the polymers present in the biomass into the smallest molecules possible (i.e., carbon monoxide and hydrogen) for it to be then synthesized into fuel molecules, thus requiring an enormous plant-specific effort.

2.3.Feedstock costs

Although capital costs may be improved with higher economies of scale, the reliability on plant size does not come without a set of complications since the costs associated with feedstock purchase and transportation correspond to almost half of the operational costs for biofuel production [13,16,35]. By expanding the overall capacity of the plant, a larger cultivated area is required for feedstock supply which, in turn, increases the contribution of biomass costs to biofuel selling prices. This expansion leads to higher logistic costs related to transportation, especially for biomasses with disperse availability and lower load densities.

3 - Opportunities for improvements

Some strategies are proposed to alleviate the drawbacks of the BtL route and, thus, improve the sustainability of the process. The previously mentioned advantages of economies of scale (see Section 0) is a strategy employed to mitigate the influence of investment costs and product yields, albeit it also impacts the expenses with feedstock. Thus, the emphasis lies in establishing a long-term biomass supply chain and optimizing the conversion technology to enhance product yields and reduce operational costs [16,36].

An important alternative to improve the economic performance of most thermochemical routes is to consider ways to expand the product portfolio of the plant on a synergistic level. As BtL processes can supply a range of by-products, usually producing more than one biofuel at a time, a diversified variety of products may reduce the production costs, which increases the plant profitability and makes biofuels more competitive [36]. The importance of by-products on the economic viability of BtL routes is evidenced even without the integration with different routes. For example, Diederichs et al. [31] observed that the credit gained by selling green gasoline and electricity responded for up to 20% of the biojet fuel minimum selling price.

An alternative to the production of an array of by-products alongside renewable fuels is the integration of emerging technologies into established processes. This strategy consists of taking advantage of the synergy between different processes and focusing on the concept of a biorefinery that includes several conversion routes that make use of all the fractions present in the biomass to produce a wide spectrum of products. The integration between utilities and services can make the process feasible even at smaller scales [36], but special conditions are necessary to obtain feasible integration scenarios. For example, Petersen et al. [39] assumed the integration of BtL routes into the sugarcane industry for South African sugar mill facilities. The authors deemed the integrated thermochemical scenarios not favorable for private investments. Alves et al. [36] studied the integration of different biofuel production configurations with different biochemicals as by-products (e.g., succinic acid, lactic acid). Among the scenarios, the authors examined the BtL route operating with woods and crops residues, either stand-alone or integrated into1G processes using sweet sorghum and sugarcane. The authors did not obtain promising results, highlighting a high risk in coproducing biojet fuel and biochemicals, which were linked to the use of 2G feedstocks, the introduction of new technologies, and the production of novel biobased products. Furtado Junior et al. [42] observed through a series of different routes integrated into a 1G sugarcane mill that, although product diversification allows the non-dependence on a single product, the high investments of some of these processes affect the viability of the overall configuration.

Bressanin et al [40] studied a similar configuration of a BtL plant integrated into a Brazilian sugarcane mill. The authors studied the use of eucalyptus during the sugarcane off-season to maintain the thermochemical processing capacity, as well as energy cane as a substitute for the conventional cane. However, the minimum selling price of the BtL fuels (biojet fuel, naphtha, and diesel) was 10-32% higher than fossil selling prices, and none of the configurations assessed were economically feasible.

The best techno-economic results were obtained by Klein et al. [7] with the production of biojet fuel by integrating the BtL route into the Brazilian sugarcane ethanol production. The authors verified that ethanol commercialization represented around 46-66% of the total revenue of these scenarios. With the additional revenue of ethanol and green gasoline, the selling price of biojet fuel decreased, thus lowering the minimum fuel selling price and improving the economic performance. Another feasible integration scenario of the study goes beyond the industrial facility: the authors also considered using the FT green diesel to supply the agricultural processes, also lowering the production costs of the biomass and the environmental impacts.

There is also the possibility of integrating the BtL route into other processes that may help improve the overall process efficiency. Some works [11,33,34] suggest introducing additional H_2 into the process to convert CO_2 into CO through the reverse water-gas shift reaction, thus improving the efficiency of the FT synthesis. Hillestad et al. [33] and Dietrich et al. [34] suggest the so-called “Power and Biomass to Liquids” (PBtL) process produces the necessary hydrogen gas by water electrolysis. The addition of this process can triple the fuel yield and convert over 90% of the biomass into fuels [33,34], but the required capital investment is 60% higher than that of the regular BtL route [33]. Also, the electricity price must be low enough to increase process economic competitiveness. The PBtL process still needs a technology push [34], as the water electrolysis technology using renewable electricity cannot compete yet with hydrogen production through fossil-based sources such as natural gas and coal [11].

Other processes that can be incorporated into the BtL route to possibly improve the product yields are the fast pyrolysis or torrefaction of the biomass [22,24,34,37]. These technologies act as biomass "pretreatment" stages, improving the fuel characteristics such as energy density, physicomechanical properties for further transportation and processing, and chemical properties [24]. Such biomass pretreatment processes also lower the requirements for the gas cleaning step due to the lower tar content of the syngas produced [22]. Moreover, biomass fast pyrolysis reactors can be built at smaller scales [43], reducing capital costs. Due to the higher energy density of bio-oil, this intermediate can also lead to lower transportation costs compared to raw biomass, thus resulting in larger optimally sized fuel production facilities and lower unit costs for fuel [44,45]. Even though many studies have evaluated the techno-economic aspects of pyrolysis and gasification alone, further studies regarding the integration of these processes into a single production chain are necessary [46].

Similar to some of the scenarios from Jiang and Bhattacharyya [32], one of the examined alternatives for the BtL route is the coprocessing of biomass alongside fossil raw materials such as coal and natural gas. Rafati et al. [11] evaluated the production of FT liquids from sawdust considering its coprocessing with natural gas. Different process configurations were analyzed (such as variation of recycle ratio and CO_2 capture) and, overall, the authors inferred that, by co-feeding natural gas and biomass, the economic performance is improved when compared to solely biomass processing. Table III-2 shows that co-feeding generally presents lower production costs. However, the authors [11] argue that none of these scenarios would be competitive with fossil-based fuels yet. In addition to coprocessing biomass and fossil materials, some studies suggest using the infrastructure of existing oil refineries to facilitate the implementation of BtL routes. The work of Holmgren et al. [35] has demonstrated that the refining of bio-syncrude along with crude oil resulted in a reduction of up to 13% of the fuel production costs compared to the stand-alone configuration. Even if the integration of biomass thermochemical plants with fossil routes does not lie entirely in the biorefinery concept, these strategies could help the market transition from full fossil-based fuels to renewable and green fuels [11]. However, it is important to keep in mind that one of the main objectives of the implementation of a renewable biofuel production route is the reduction of environmental impacts, especially GHG emissions. This integration into the fossil production chain may be more economically attractive, but it may not be the most sustainable solution in the long run.

With the environmental concern as one of the main drivers for advanced biofuel production, another possibility of integration is with carbon capture systems. During the syngas production and cleaning stages, a considerable amount of carbon dioxide is produced and not consumed in the downstream processes [34]. Some studies propose to capture this carbon stream as well as other emissions along the process. Even though such carbon emissions are considered biogenic, by capturing them, it is possible to achieve negative net GHG emissions in the process. Kempegowda et al. [37] observed slightly worse economic results (reduction of 4% in IRR) with the implementation of a carbon capture and storage (CCS) system with higher production costs when compared with the base scenario without the implementation of CCS. The lower economic feasibility of adding a CCS system must be analyzed on a wider scope when more subsidies and incentives for improved environmental performance are contemplated.

4 - Case study for Brazil

The overall objective of this case study is to provide a preliminary assessment seeking viable conditions to obtain advanced fuels in Brazil, with a focus on evaluating the techno-economic performance of thermochemical technologies. The main hypothesis is that the BtL process has the potential to produce advanced biofuels in a scenario integrated into the current Brazilian sugarcane industry. For the current market context, sugarcane is the main biomass adopted for different biorefinery alternatives, mainly due to its large availability and well-developed sugar and ethanol production chain from the sugarcane juice (first-generation ethanol).

Therefore, the present study performs a techno-economic analysis of scenarios using the Virtual Sugarcane Biorefinery (VSB) [47], a framework of different software and electronic spreadsheets developed at the Brazilian Biorenewables National Laboratory (LNBR), which allows the evaluation of different biorefinery configurations. For the economic evaluation of the scenarios, a discounted cash flow analysis was carried out considering a greenfield project.

The main metrics adopted are the net present value (NPV), the internal rate of return (IRR), as well as the biofuel production costs. The assumptions of this analysis are presented in Table III-3, with typical values for the Brazilian sugarcane sector [48].

Table III-3 – Main assumptions of the techno-economic assessment

Item	Value	Reference
Expected project lifetime	25 years	[47]
Discount rate	12% per year	[47]
Reference date	December 2019	Assumed
Exchange rate	R$ 4.03 = 1 US$	[49]
Depreciation	10 years, linear	[47]
Electricity price	US$ 54/MWh	[50,51]
Working capital	10% of CAPEX	[47]
Taxes	25% + 9% of taxable income	[47]
Maintenance	3% of CAPEX	[52]
Insurance and others	0.7% of CAPEX	[52]
Ethanol price	0.43 US$/L	[53]
Biojet fuel price	0.53 US$/L	[54]
Green gasoline price	0.45 US$/L	[54]

4.1.Agricultural stage

The simulations of the agricultural phase were performed using the CanaSoft model, a platform developed as part of the VSB framework [47]. This platform considers all agricultural operations (from soil preparation to biomass transportation to the mill), taking into account a variety of inputs such as machinery, agricultural implements, trucks, and labor. With an optimal and current scenario available for new sugarcane biorefineries, the full mechanization of the agricultural stage was considered. Table III-4 presents the most important parameters for this stage. It is important to note that not all straw produced can be harvested since a fraction must remain on the fields to maintain soil quality [20]. Thus, the process collects only 50% of the available straw on the field on a second-pass straw harvesting operation. This collection expressively increases the lignocellulosic material available to the thermochemical process.

Table III-4 - Main parameters adopted in the agricultural simulations

Agricultural parameters	Value	Unit	Source
Sugarcane yield	80	TC/ha	[55]
Straw recovery	2.4	t_{db}/ha	Assumed
Straw recovery fraction	50	%	Assumed
Straw recovery method	bales	-	Assumed
Mean transportation distance	36	km	Calculated
Sugarcane stalks production cost	21.67	U$/tonne	Calculated
Sugarcane straw production costs	27.44	U$/tonne	Calculated

db: dry basis; ha: hectare; TC = tonnes of cane

4.2. Industrial stage

Mass and energy balances of the industrial phase of the integrated biorefinery were obtained from the Aspen Plus® process simulator version 8.6 (AspenTech, Bedford, MA, USA). Figure III-1 depicts a simplified flowchart of the industrial process, while Table III-5 presents a summary of the main operational parameters of the biorefinery. A detailed description of the simulation can be found on the Supplementary Material.

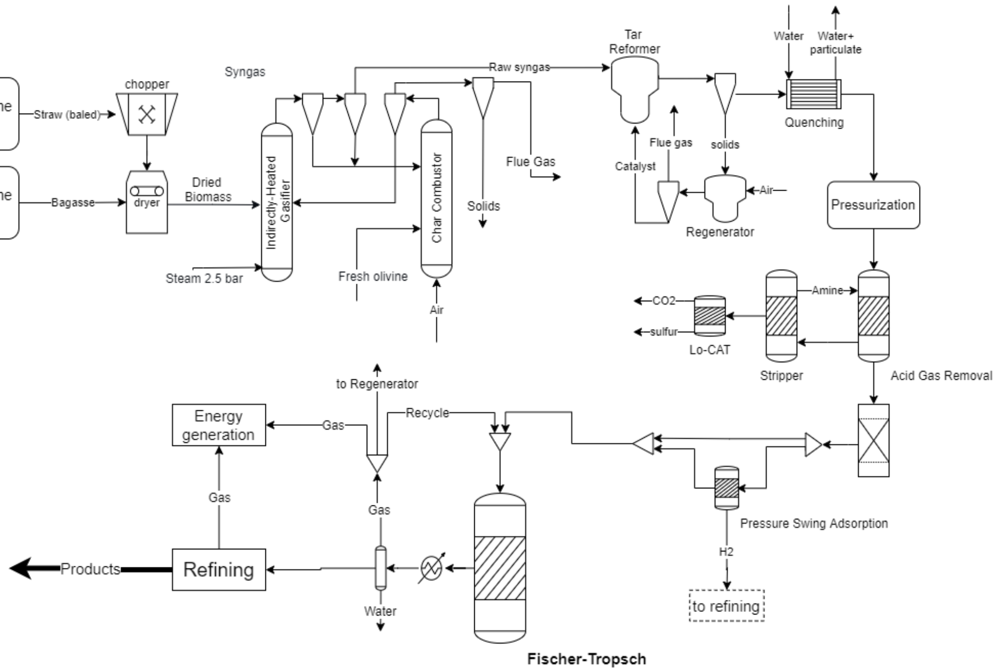

Figure III-1 – Simplified process flowchart (adapted from Bressanin et al [40]*)*

Table III-5 - Main parameters for the industrial stage of the base case

Industrial Parameters	**Value**	**Unit**	**Reference**
Overall process			
Total sugarcane processed	4	Million TC	Assumed
Operational days	200	Days/year (season)	
	330	Days/year (season + off-season)	
Reception and cleaning			
Electricity demand (conveyors and fans)	0.692	kWh/tonne	[47]
Extraction			
Efficiency of sugar extraction in the mills	96	%	
Amount of imbibition water	280	kg/TC	
Bagasse moisture	50	%	
Fermentation/distillation			
Fermentation efficiency	90	%	
Wine ethanol concentration	80	g/L	
Biomass preprocessing (thermochemical process)			
Target biomass moisture content	10	wt%	[52,56]

Electricity demand (sieves, choppers)	3.73	kWh/tonne	[47]
Heat demand (dryer)	1.5	MJ/kg$_{\text{evaporated water}}$	Calculated
Gasification			
Indirect gasifier temperature	870	°C	Assumed
Pressure	2.5	bar	[52]
Steam-to-biomass ratio	0.4	wt% (wb)	Assumed
Syngas cleaning			
Solid removal on cyclones	99	%	[52]
Tar reforming temperature	910	°C	[56]
Tar reforming steam consumption	0.28	kg$_{\text{steam}}$/kg$_{\text{syngas d.b}}$	Calculated
H_2/CO ratio after reforming	2.15	mol/mol	Assumed
Water for quenching	1.9	kg$_{\text{water}}$/kg$_{\text{syngas}}$ (wb)	Calculated
Amine consumption on AGR	1.15	kg$_{\text{amine}}$/kg$_{\text{syngas}}$ (wb)	Calculated
Electricity demand (pressure rising)	0.19	kWh/m$^3_{\text{gas}}$	Calculated
Fraction of syngas directed to PSA	1.3	wt%	Calculated
FT synthesis			
Reactor temperature	200	°C	[56]
Single-pass carbon conversion	40	%	[56]
Recycle ratio	0.3	wt%	Assumed
Refining	-	-	[57]
Power generation			
Boiler pressure	90	bar	[47]
Process steam demand	420	kg/TC	Calculated
Electricity demand	53	kWh/TC	Calculated
Process output			
Biojet fuel	23.05	L/TC	Calculated
Ethanol	87.69	L/TC	Calculated
Green gasoline	8.63	L/TC	Calculated
Surplus electricity	98	kWh/TC	Calculated

AGR: acid gas removal; PSA: pressure swing adsorption; TC: tonnes of cane; wb: wet basis

The operational parameters were obtained from the literature, considering an optimized autonomous ethanol distillery as the main plant for the integration with the thermochemical plant. The base ethanol distillery operates during the sugarcane season (200 days/year) crushing 4 million tonnes of sugarcane/year, producing hydrous ethanol (93 wt%) as the main product. The configuration of this process considers the most modern equipment and setups, such as high-pressure boilers, reduced process steam consumption, and electric mill drivers. Further detailing of this modernized distillery is available elsewhere [47].

In the proposed scenario, after the 1G process (ethanol production), the bagasse from the mill and the straw collected from the field in the form of bales are directed to the thermochemical section of the plant. During the sugarcane season, part of the lignocellulosic material (bagasse and straw) is stored to supply material during the off-season operation. The BtL route begins with a pretreatment stage of the biomass. The straw is unbaled, chopped, and sieved, and both straw and the bagasse are dried to 10 wt% moisture in a direct-contact steam rotatory dryer [58,59].

The dried biomass is gasified with a low-pressure indirectly-heated circulating fluidized bed gasifier. This configuration is usually less capital-intensive than alternatives such as a directly heated gasifier, mostly due to the reactor itself and the absence of an air separation unit [40,59]. Besides that, fluidized beds present higher carbon conversion efficiencies, good heat, and material transfer, and can be easily scaled up [60]. The gasification process conditions and calculations were adapted from the works of Dutta and Philips [61], Dutta et al. [52] and Bressanin et al. [40], with superheated steam (310 °C and 2.5 bar) as a gasifying at a ratio of 0.4 tonnes of steam per tonne of dry biomass. Cyclones at the exit of the gasifier separate 99.99% of the olivine and char present in the syngas and 90% of residual fines are removed in a secondary gasifier cyclone. This solid is fed to the char combustor, and the heat generated in the combustor is transferred to the gasifier by the recirculation of the olivine [52]. This heat exchange leads to a thermal equilibrium between the gasifier and combustor (870 °C and 980 °C, respectively) [52]. The gasifier pressure is assumed to be 2.3 bar, and the char combustor pressure is 2 bar.

The syngas clean-up was based on a series of references [52,56,61] and consists of tar reforming, cooling/quenching, acid gas removal (AGR), pressurization, and pressure swing adsorption (PSA).

The tar reformer is an entrained-flow fluidized catalytic reactor (Ni/Mg/K catalyst). At this stage, light hydrocarbons are converted to CO and H_2 while NH_3 is broken into N_2 and H_2. For these reactions, the target conversions presented by Dutta et al. [52] and Zhu et al [59] were used. Since the catalyst has significant water-gas-shift activity [52], steam is injected into the tar reformer to shift the equilibrium and adjust the H_2/CO ratio at the FT reactor to the optimum for biojet fuel production (ratio of 2.15). Excess air (20%) is fed into the catalyst regenerator reactor to provide oxygen for the combustion of carbon deposits (coke) of the catalyst particles, regenerating their catalyst activity. The circulating catalyst between the reformer and the regenerator provides energy for the system. Supplemental unconverted syngas from the FT synthesis area is also supplied to the regenerator to help supply the necessary energy.

Syngas is cooled to around 60 °C, and a scrubbing system is employed to further cool the gas and to remove particulates, ammonia, and residual tars [52]. Quench water circulation rate is 1 liter per cubic meter of gas [52]. Due to the low-pressure gasifier, the syngas is compressed to around 30 bar using a five-stage centrifugal compressor with interstage cooling [62].

The removal of sulfur and CO_2 is performed by an amine-based absorption system consisting of an absorber, a stripper column, a flash separator, heat exchangers, and a LO-CAT® sulfur recovery system. The acid gas is removed by chemical reactions with amine methyl-diethanolamine (MDEA) [63]. The LO-CAT® system isolates H_2S from CO_2 and converts it to solid sulfur. A final step with zinc oxide (ZnO) gas polishing is used as a catalytic absorbent for sulfur removal, achieving a sulfur content below 50 ppb [62]. A small percentage of clean syngas is departed to the PSA unit to isolate a stream of hydrogen to be used in hydroprocessing facilities.

For the present study, FT synthesis was conducted on a tubular fixed bed reactor, with cobalt catalyst and inlet pressure and temperature of 25 bar and 200 °C, respectively. The tubular fixed bed reactor was selected because it is well suited for wax production due to simple liquid/wax removal and simpler operation [40,56]. The FT operating conditions were chosen to maximize the production of liquid fuels. It was assumed a per-pass carbon conversion of 40% [56], and the product distribution follows the ASF distribution. Detailed steps of the necessary calculations are described by Swanson et al. [56].

The outlet of the reactor is cooled to under 40 °C, with the recovery of liquid water and hydrocarbons in a gas/liquid knock-out separator. Part of the unconverted syngas is directed to the catalyst regenerator (tar reforming) and another part is directed to a gas turbine for power and steam generation [7]. The remaining syngas is recycled to the FT reactor. A refinery design proposed by Klerk [57] aiming to maximize the production of jet fuel with the production of additional green gasoline was selected.

The biorefinery was conceived to be energy self-sufficient, operating without any additional external energy sources. The energy generation of this integrated plant is different from the stand-alone 1G process. While in the current ethanol production, bagasse combustion supplies the energy demand of the plant, in the integrated configuration, the thermochemical process supplies energy to the entire plant. Thermochemical plants are known to generate significant amounts of energy in the form of process steam produced through the cooling of the various high-temperature process streams [7]. Different process integrations were assumed to enable the generation of heat and steam. The supplementary material contains a more detailed description of the assumptions for the process and simulation, besides information pertinent to costs and investment estimations.

Table III-5 also brings the production output of each product. Ethanol has the largest share of the production since it is produced by the 1G facility, a mature and well-developed process with higher efficiencies and conversions. On the other hand, the thermochemical process is less mature and presents lower yields [30,34]. Finally, since the focus of the process is to maximize biojet fuel production, green gasoline represents only a small fraction of the total production. Besides these fuels, there is also a significant production of surplus electricity.

4.3.Techno-economic results

Table III-6 presents the main economic results of the base case. Before discussing the economic feasibility of the plant, it is important to highlight the contribution of each product to the revenue. As shown in Table III-3, the output volume highly influences the revenue. Since ethanol is the main product in terms of the final output, it has the largest participation in the revenue, followed by biojet fuel. As identified by Klein et al. [7] and Bressanin et al. [40], there is an expressive dependence on the ethanol revenue, so the commercialization of ethanol can make the bio-thermochemical integrated facility more profitable.

Table III-6 - Main economic results of the base case

Total investment cost	625.30	MM U$
Fixed capital investment	568.45	MM U$
Annual operational costs	140.43	MM U$
Total production costs*		
Ethanol	0.394	U$/L
Green gasoline	0.415	U$/L
Biojet fuel	0.487	U$/L
Electricity	47.937	U$/MWh
IRR	10.6	%
NPV	-57.16	MM U$
Participation on revenue		
Ethanol	64.2	%
Green gasoline	4.2	%
Biojet fuel	13.1	%
Electricity	18.5	%

*Based on capital and operational costs

The limited contribution of the thermochemical fuels combined with their lower outputs is also linked to the current efficiency of the BtL process. As mentioned in previous works [30,34], the BtL process has low carbon conversion, with around 70% of the total carbon present in the lignocellulosic biomass being transformed into CO_2. In the present study, only around 15% of the carbon initially present in the bagasse and straw was converted into biojet fuel and green gasoline. The overall energy efficiency of the process, calculated by the ratio between the total energy output (fuels plus electricity) and the energy input (energy present in biomass in the form of lower heating value), achieved a value of 50%, pointing out that this scenario still needs improvement.

The main problem with the current configuration is the high consumption of energy and heat by the 1G mill. According to Furtado Junior et al. [42], the conventional process of ethanol and sugar production is responsible for most of the heat and electricity consumption, and this is especially true for the current integrated process. Since the available lignocellulosic biomass (bagasse and straw) obtained during the season period (200 days) must be used during the entire year (330 days, season and off-season), a compromise is necessary to balance thermochemical fuel production and power generation for the 1G mill. Only 30% of the unreacted syngas leaving the FT reactor is recycled back to the reactor, and most of the gas is directed to the combined cycle, mainly to meet the steam demand. The necessity to prioritize steam generation hinders the production of biofuels and the result is a less energy-efficient process. Furtado Junior et al. [42] also observed that, if all bagasse from a sugarcane mill was destined to the thermochemical route, the cogeneration cycle would not be able to supply the process energy demand, in a way that part of the syngas must be used to meet this requirement. Therefore, the produced syngas was diverted to energy generation before FT conversion, and approximately 20% of the gas was destined for electricity and heat generation.

By comparing the results obtained in this assessment with those obtained from a previous study [40], the difference in efficiency can be perceived since the previous work managed to reach global energy efficiencies above 50% for a similar configuration. However, the main contributor to this result is the availability of lignocellulosic biomass since the configuration of Bressanin et al. [40] considered the acquisition of eucalyptus to feed the BtL route during the off-season to maintain a higher processing capacity. With a higher biomass flow being fed to the BtL process, more syngas is produced and it is possible to meet the 1G steam demand without compromising fuel production. According to Furtado Junior et al. [42], by prioritizing the FT synthesis, the overall efficiency of the process increases, and, thus, the increase in fuel output brings benefits.

Despite this low carbon conversion into biofuels, the current configuration achieves an IRR close to the range of the minimum required (around 12% per year for the sugarcane industry in Brazil). This result indicates that the high participation of ethanol and electricity in the revenue may alleviate the impact of low BtL yields on the integrated facility. However, some caution is necessary when analyzing the integration between the BtL route and 1G mills. The production of ethanol may help increase the revenue but, on the other hand, if the lignocellulosic biomass supply is not enough as was observed in the present study, the heat and electricity demands of the integrated process may compete with fuel generation.

The IRR of the base case of the present study (10.6% per year) is closer to those obtained by Bressanin et al. [40] for a similar configuration of a BtL route integrated into a Brazilian sugarcane mill. When compared to the study of Klein et al. [7], this work presents lower IRRs for the integrated sugarcane mill/thermochemical process. Our IRRs, however, were at least 30% higher than those obtained by the different integrations proposed by Alves et al [36]. Our economic results suggest that the integration and product diversification strategies require high investments [42] especially with the use of 2G feedstocks for novel biobased products [36]. Thus, relying on well-established products (such as fuels and electricity) may be a better option to improve the economic performance and also to decrease the risks of the project investment.

To better evaluate the results presented in Table III-6, the production costs breakdown in Figure III-2 shows that the costs associated with biomass production/transport and capital investment are the largest components of the production costs.

As presented in Figure III-2, the CAPEX of the BtL plant represents the largest share of the production costs. Many studies corroborate the fact that the fixed capital expenses of a large-scale thermochemical biorefinery represent most of the production costs, adding up to above 30% of the production costs [12,41]. The breakdown of the capital costs shows that the costs associated mainly with the thermochemical process correspond to over half of the CAPEX (namely gasification, syngas cleaning, and fuel synthesis). The 1G mill technology, however, represents only 21% of the CAPEX, similar to that observed by Bressanin et al. [40], with the 1G technology responding up to 20% of the total CAPEX. Furtado Junior et al. [42] also demonstrated the higher participation of the BtL process in the total capital investment, with this technology responding for 70% of the investment. The technology for 1G ethanol production is cheaper than the BtL technology in terms of equipment costs, and it is also a well-established route in Brazil. 2G thermochemical plants, however, are more complex and expensive to build [40].

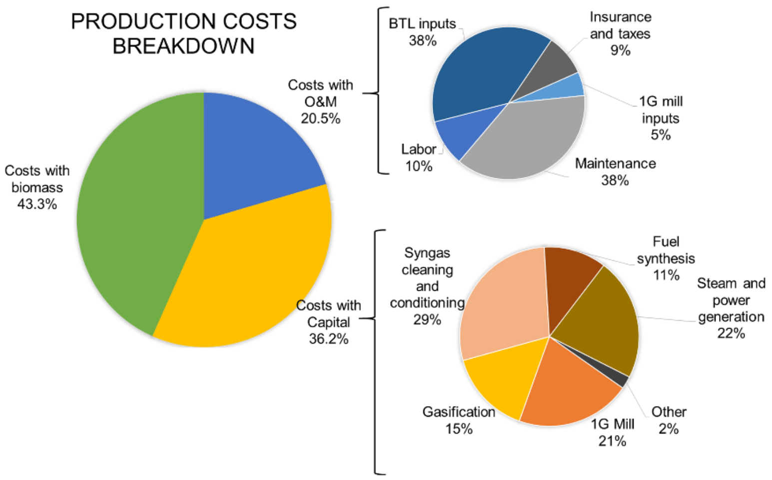

Figure III-2 – Fuel production cost breakdown of the industrial plant

Many studies indicate that the costs associated with feedstock can add up to almost half of the operational costs [13,16,35], which can be observed in Figure III-2. The biomass production costs are due to the relatively high capacity of the present configuration: a thermochemical biorefinery with a yearly processing capacity of 4 million tonnes of biomass could be understood as too ambitious and of too much large scale for Europe and North America standards, where many biomass production sites are widespread in large territories [37,64,65]. However, biomass availability is not a constraint in the Brazilian context, especially for sugarcane production. The Center-South region of the country presents a dense sugarcane production distribution and responds for the largest part of the production (almost 90% of the total Brazilian production). Price fluctuations of sugarcane bagasse and straw may affect biomass availability according to the seasonal demand for thermoelectricity generation in the same region of the country which, in turn, is affected by the rainfall regime in this region [20].

Nearly 10% of the sugarcane milling facilities have capacities of over 4 million tonnes of sugarcane per year [19]. Nonetheless, Brazil has mills with annual capacities of up to 10 million tonnes. However, considering the high share of biomass in the overall production costs, this importance should be carefully analyzed, especially if the economies of scale are to be envisioned. As for the other operational expenses, the high maintenance costs are linked to the equipment costs and the total CAPEX. The high expenses on inputs for the thermochemical process are, in turn, associated with the high costs and consumption rates of catalysts, especially the cobalt catalyst for the FT synthesis.

4.4.Possible improvements

The first possible means to improve the viability of the current BtL configuration is to explore the benefits of the economies of scale. Many studies indicate that the increase in the plant scale can lead to better economic results, provided that the costs with biomass acquisition are kept under control [12,13,16,30,32,35].

Therefore, Figure III-3 shows the influence of the total annual capacity of the plant on the IRR and NPV of the project. The positive effect of the increased industrial scale is seen for milling capacities up to 8 million yearly tonnes of sugarcane. For this plant size, the process can reach an IRR in the range of feasibility and a maximum for the NPV. However, for plants above this size, the operating costs with biomass production, collection, and transportation start to deteriorate the incremental benefits from increasing scales. For milling capacities over 8-10 million tonnes per year, the IRR slightly decreases while the NPV presents a sharp decrease.

The raise of expenses on feedstock acquisition and logistic fees may limit the benefits from the economies of scale: there is a threshold for the size of a thermochemical plant above which the operational and logistic costs surpass the profits from increased productivity. Such a threshold, therefore, raises the necessity to focus on lower feedstock costs and optimized agricultural production.

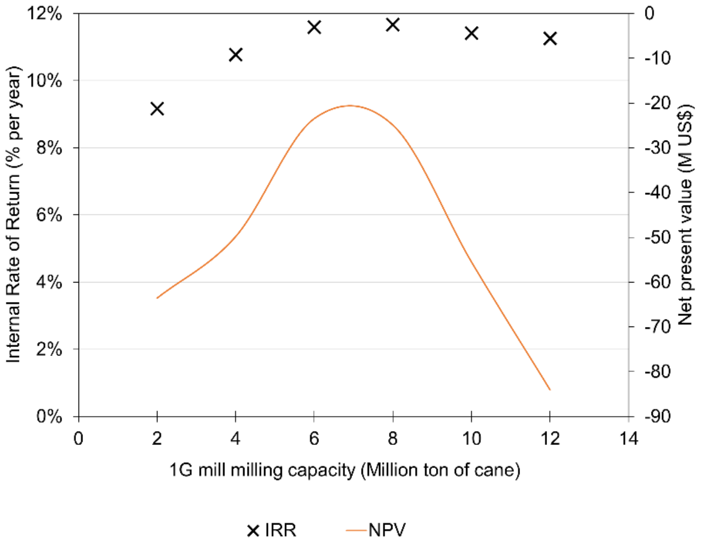

Figure III-3 - Effect of increased industrial scale on internal rate of return (IRR)

As mentioned previously (see Section 4.3), large-scale biorefineries with annual milling capacities in the range of 4-8 million tonnes, while not numerous, are indeed a reality in Brazil [19]. Therefore, for further analysis, the capacity of the proposed plant will be set to 8 million tonnes of sugarcane annually. Considering that the scale of the largest sugarcane mill in the Southeast region of Brazil is of this magnitude (around 10 million tonnes of sugarcane per year), this plant size is plausible and will be evaluated as a "best-case scenario". The current configuration of a yearly 8 million tonnes capacity of sugarcane may yield economic results just on the lower limit of viability. However, for this process to be economically attractive, it is necessary to find ways to further improve its performance.

The maturity of the technology could reduce the costs of industrial equipment and ensuing fixed capital expenses, since CAPEX can be reduced by the maturity of equipment manufacturing in the country [40], thus avoiding the extra costs related to the location factor.

Lower biomass costs could also be achieved with, for example, improvements in biomass productivity and changes in harvesting technologies and biomass transportation [66]. Also, external factors could influence the project, such as economic scenarios with varying product market prices. Figure III-4 shows the influence many of these factors have on project viability (measured by the IRR), setting as ± 30% the higher and lower limits of each parameter.

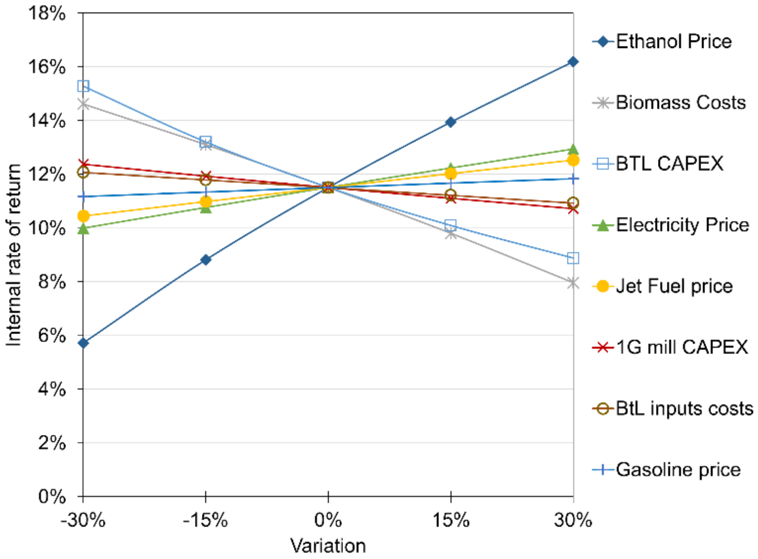

Figure III-4 - Influence of different parameters (± 30% variation) on the internal rate of return (IRR)

Ethanol price has the greatest influence on the IRR (positive correlation) since it is the main product in terms of mass output (Table III-5) and participation in the revenue of the integrated scenario (Table III-6). Thus, changes in its price should lead to great variations in the economic performance of the process. The same can be said about biomass costs, due to the size of the plant (8 million tonnes of sugarcane per year). The effect of this factor, however, is opposite to that of the ethanol price: with increasing biomass costs, the plant becomes less viable.

Electricity and biojet fuel prices also present a significant impact on the economic viability, in the same manner as the influence of ethanol price, albeit less prominent. However, the green gasoline price is less influential in the overall viability of the plant since this product represents a small share of the overall revenue (Table III-6).

Another important factor for the viability of the project is the capital investment, which raises an important discussion since the variation of the BtL plant CAPEX presents a larger influence than the changes in the sugarcane mill CAPEX. The reason for the larger influence of the BtL CAPEX is that the thermochemical process responds for the largest sum of the capital investment, while the sugarcane mill technology is significantly cheaper. As a comparison, for the current configuration, the capital investment for the 1G mill is in the order of US$ 25-30 per tonne of sugarcane processed in a year (wet basis), while the investment for the BtL process per tonne of lignocellulosic biomass processed yearly is above 500 US$ (dry basis).

Considering a rigorous minimum acceptable rate of return (MAAR>12% per year), with one parameter varying each time as shown in Figure III-4, the variation of biomass costs, ethanol price, and BtL route CAPEX may lead to a more attractive return for the investment, with an IRR above 15%. Aiming to further improve the IRR and identify more feasible scenarios for the project, Figure III-5 shows the influence of two parameters jointly on the IRR.

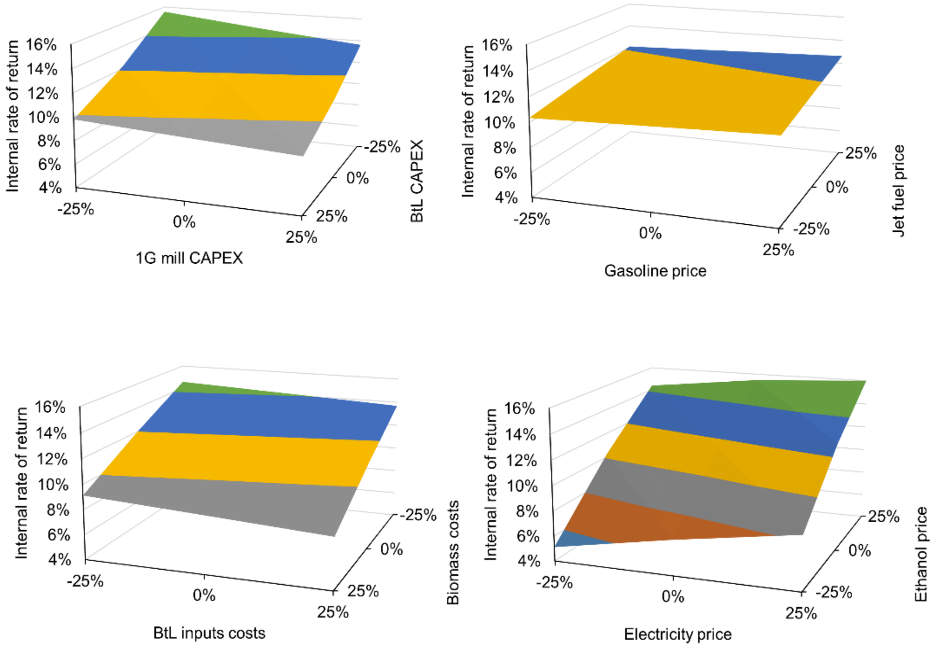

Figure III-5 – Influence of combined parameters on the internal rate of return (IRR)

The results shown in Figure III-5 can help direct the selection of the parameter values that would lead to the best economic performance. For example, the prices of the outputs (ethanol, biojet fuel, green gasoline, and electricity) should be maximized, while the other parameters should be minimized. The underlying problem is that variations of ± 25% may not represent statistically possible results for each of these factors. To illustrate that, ethanol price is not likely to vary to this extent, albeit possibly with some unexpected economic scenarios. Thus, it is important to consider the historic variation of these prices and costs to evaluate the possible range of variation these parameters can realistically have, which is performed in Table III-7.

Over the past 10 years, ethanol prices [53] varied from 0.30 U$/L to up to 0.57 U$/L. However, statistically, there is a 50% probability for this price to be in the range of 0.40-0.46 U$/L which, in turn, represents a variation of -8% to +7% of the median value. The same logic applies to the historic variation of the gasoline price [54], by considering the statistical distribution (median, standard deviation) of the historic variation of these values. The electricity price follows an analogous path; however, the historic variation considers an average of the variation of the direct price [51] and the auction price of electricity [50]. The range of the costs with the BtL route inputs is estimated by considering the variation of the main input – the FT metal catalysts [67] – that represents almost 40% of the total input costs calculated for the thermochemical plant. As for the CAPEX, there is no historic variation for these parameters. The possible variations are, in reality, associated with the uncertainties and the accuracy of the estimation of the total capital cost. According to Dutta and Phillips [61], for this kind of conceptual design, the uncertainties are in the range of -10% to +30%. Thus, this variation range was used for the CAPEX estimation.

This kind of sensitivity analysis can also help compensate for simplifications and considerations made during the elaboration of the base scenario. For example, it would be expected that the creation of a large-scale plant consuming sugarcane influences the local demand of this feedstock and affects its price. This case is contained in the range of variation of the feedstock price. Another possible effect is the existence of policies and incentives for biofuels (such as RENOVABIO [4]). This kind of incentive can be described with the increasing price of biofuel, which is linked to the revenue of the plant.

Table III-7 – Possible variation range for each parameter for the scenario analysis

	Variation		Period	Source
Gasoline price	-5%	+6%	2002-2019	[54]
Sugarcane cost	-5%	+7%	2008-2019	[68]
Ethanol price	-8%	+7%	2004-2019	[53]
Jet fuel price	-16%	+15%	2002-2019	[54]
Electricity price	-13%	+27%	2003-2019	[50,51]

CAPEX BtL	-10%	+30%	-	[61]
CAPEX 1G mill	-10%	+30%	-	[61]
BtL inputs	-50%	+57%	2009-2019	[67]

With the variations of each parameter described in Table III-7, the results for different possible scenarios are presented in Table III-8. The construction of the scenarios considers two possible plant capacities (4 and 8 million tonnes of sugarcane per year) and a group of possibilities named in Table 8 as pessimistic, base, and optimistic. The base scenarios consider the average value of each parameter. As for the pessimistic scenarios, the costs (CAPEX, inputs costs, and biomass costs) are maximized whereas the product prices are minimized. The optimistic case considers the opposite, with minimum costs and maximum product prices. An over-optimistic case is also simulated, which assumes a variation on the calculation of the total CAPEX to assess the best possible conditions for the technology.

Since the CAPEX estimation for the thermochemical section of the plant presents different equipment whose prices are not available at a Brazilian source, many of these costs were collected from foreign sources [52,56,61,63] and corrected by using a “Process Plant Location Factor” [69] of around 1.3 – which means an additional 30% expense over the imported equipment costs – to account for the transport and services related to the import and setup of such equipment. This over-optimistic scenario assumes this location factor is equal to 1.0, assuming the development of this technology in Brazil without the need of importing them from other countries.

The pessimistic cases for both capacities are extremely unfeasible and result in an IRR below 10-12%. The high costs associated with an increased CAPEX and lower revenues due to low product prices are responsible for this result. For the base case, both capacities land on the lower range of economic viability (IRR of 10-12%). When optimistic and over-optimistic scenarios are taken into account, both capacities present IRR values well above the minimum, exceeding 15% per year. Therefore, under favorable scenarios, the BtL route may be economically feasible in a Brazilian context.

Table III-8 – Assumptions and economic results for each scenario

Milling capacity	**4 Mtonnes of cane/year**				**8 Mtonnes of cane/year**			
Scenario	Pes	Base	Opt	Over opt	Pes	Base	Opt	Over opt
Assumptions								
Biomass costs	+	0	-	-	+	0	-	-
Prices	-	0	+	+	-	0	+	+
CAPEX	+	0	-	-	+	0	-	-
Thermochemical inputs costs	+	0	-	-	+	0	-	-
Importation/ Location factor	0	0	0	-	0	0	0	-
IRR (%)	2.7	10.6	16.2	19.2	3.4	11.5	17.4	20.5

+: maximum value; -: minimum value; 0: median value; Opt: optimistic scenario; Over opt: over optimistic scenario; Pes: pessimistic scenario.

5 - Conclusions

There is still room for improving the feasibility of the BtL route for the large-scale production of biofuels. Brazil presents many of the factors that can help the implementation of this process, such as an existing biorefinery infrastructure with wide biomass availability, part of which is already available in the production site. The integration of the thermochemical process into a sugarcane mill/1G ethanol distillery provides the BtL route with a well-established infrastructure, and the income generated with the commercialization of ethanol may improve the economic performance of the BtL plant for the production of biojet fuel.

However, the high fixed capital investment (which represents over 30% of the biofuel production costs) due to high expenses with equipment and technologies is still an obstacle. Thus, reduction in equipment costs and import fees are still required, perhaps by developing these technologies internally in the long run. For instance, if the technology were produced inside the country (location factor = 1), the IRR would increase 33% from the base value. An eventual reduction of 10% on the total equipment costs of the thermochemical route would improve the IRR of the project by over 10% per year.

In addition to this technological improvement, some aspects of the market status could enhance the feasibility of the process. The reduction in biomass costs and the increase in ethanol prices combined could result in an IRR of nearly 15% per year. Incentives and subsidies must be offered to biofuel production to improve the competitiveness with fossil-based fuels, such as the National Biofuels Policy (RenovaBio), already in motion in Brazil. This mechanism forces the distributors to prioritize the commercialization of a minimum required amount of biofuels via the generation of CBIO (Decarbonization Credit), a tradeable financial asset issued by the biofuel producer [3].

The current paper highlighted and quantified some of the bottlenecks for the implementation of BtL routes, with an emphasis on biojet fuel production. The integration between the Gasification/FT technology and a Brazilian sugarcane mill is promising, given some aspects such as equipment costs and market conditions are favorable and can be improved in the future. Further studies are necessary to improve the process, such as life cycle assessment of the technologies presented in the scenarios, increasing the process overall efficiency by heat integration and the use of additional biomass sources, and also estimating the potential additional revenues from carbon credits obtained with thermochemical biofuels. The evaluation of a stand-alone plant is also necessary, taking into account the logistical aspects since biomass costs are one of the main factors for production costs.

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Author contributions

Conceptualization, H.R.G., M.D.B.W; methodology, H.R.G., M.D.B.W. J.M.B., B.C.K., M.F.C.; validation, H. R. G., M.D.B.W., J.M.B., I.L.M.; formal analysis, H.R.G., M.D.B.W., J.M.B., I.L.M.; data curation, H.R.G., M.D.B.W., J.M.B.; writing—original draft preparation, H.R.G., M.D.B.W.; writing—review and editing, H.R.G., M.D.B.W., J.M.B., I.L.M., B.C.K., R.M.F; supervision: M.D.B.W., A.B., R.M.F. All authors have read and agreed to the published version of the manuscript.

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Chapter IV - Standalone and Integrated GFT scenarios

The second article was accepted and published on the journal Chemical Engineering Transactions, vol. 92 on June 30, 2022. This paper originated from a work presented on the International Conference on Biomass 2022, held on Naples, Italy from June 5-8, 2022. This short work focusing on expanding the paper from Chapter III - to include environmental analysis and comparison of the standalone and integrated configuration of the BtL route.

Techno-Economic and Environmental Assessments of Thermochemical Routes Integrated into the Brazilian Sugarcane Industry for the Production of Renewable Jet Fuel

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Environmental agreements and international concerns on greenhouse gas (GHG) emission reduction policies have pushed for the search for economically viable ways to produce sustainable biofuels, such as renewable jet fuels to decrease fossil fuel-based GHG emissions in the international flight sector. The gasification of lignocellulosic biomass followed by catalytic conversion (Fischer-Tropsch reactions) in Biomass-to-Liquids (BtL) plants is a solution to this demand. However, this process still presents some techno-economic setbacks. Brazil is one of the major players in the biofuels market worldwide, and its existing biorefining infrastructure from the sugarcane sector can be used as the basis to support the large-scale implementation of such advanced biofuel production routes. This study compares a standalone BtL plant configuration to a scenario integrated into a sugarcane mill/ethanol distillery. Both scenarios operate by processing sugarcane bagasse and straw and, through a techno-economic analysis aided by a simulation framework (the Virtual Biorefinery), it was possible to observe that the integration was able to improve the economic performance of the BtL route. A greenfield standalone plant could not achieve economic feasibility, but the integrated configuration achieved internal rates of return of 10-12% per year. Some aspects may improve the viability of BtL plants, such as logistic chain optimizations to reduce costs with feedstock acquisition and the consideration of environmental policies and incentives to help increase revenue.

1 - Introduction

The interest in large-scale renewable and sustainable fuel production has grown worldwide as a way to mitigate the effects of climate change. This is particularly the case for fuels used for long-haul transportation, such as jet fuel, which still do not have a consolidated renewable alternative. The thermochemical Biomass-to-Liquids route (BtL) is one of the most likely alternatives to supply this demand (IRENA, 2017). This route can produce green diesel, green gasoline, and biojet fuel with similar characteristics to fossil fuels with the benefit of lower pollutants emission (Rafati et al., 2017). However, high equipment costs (Dimitriou et al., 2018) and dependence upon the biomass supply chain (Motta et al., 2018) make it difficult to successfully implement this route for large-scale applications. In order to increase its efficiency, the gasification could be integrated into other industrial processes (Peres et al., 2013). The Brazilian sugarcane industry presents a well stablished technological infrastructure with large amounts of sugarcane bagasse and straw, lignocellulosic residues available for further valorisation (Leal and Hernandes, 2020). This market can act as a more favourable environment to develop these BtL processes.

The overall objective of this study is to evaluate thermochemical technologies to obtain advanced biofuels, focusing on their economic performance and environmental impacts. This evaluation centers around the large-scale production of biojet fuel in BtL plants (containing gasification and Fischer-Tropsch (FT) conversion units) either integrated into a sugarcane mill/ethanol distillery or working as standalone facilities. The main hypothesis is that the process of gasification/FT conversion has the potential to be a suitable route to produce biojet fuel in a scenario integrated into the Brazilian sugarcane industry.

2 - Methodology

Considering the well-stablished infrastructure and consolidated market in Brazil, sugarcane is the main biomass adopted for different biorefinery alternatives, taking into account the ethanol production chain from sugarcane juice (first-generation (1G) ethanol) and the use of bagasse and straw as second-generation feedstock. Two scenarios were evaluated to compare the effects of such integration on the selected technological route, and both are presented in Figure 1. The first scenario is a standalone (SA) thermochemical BtL plant with a processing capacity of 1 Mt of dry lignocellulosic material (LCM) per year. This configuration operates 330 days/year by purchasing sugarcane bagasse and straw from surrounding sugarcane mills. The configuration of this thermochemical process and the biomass characteristics are explained in a previous study (Guimarães et al., 2021). The second case is the same configuration of the BtL plant and integrated (INT) into a 1G ethanol distillery producing hydrous ethanol (93 wt%). This 1G distillery is considered to be the most modern configuration, with further detailing available elsewhere (Bonomi et al., 2016). The mill operates during the sugarcane season (200 days/year), and the bagasse from the mill and the straw collected from the field in the form of bales are stocked and directed to the integrated thermochemical section, which operates 330 days/year. A processing capacity of around 5 Mt of sugarcane per year was chosen to maintain the processing capacity of 1 Mt of dry LCM per year.

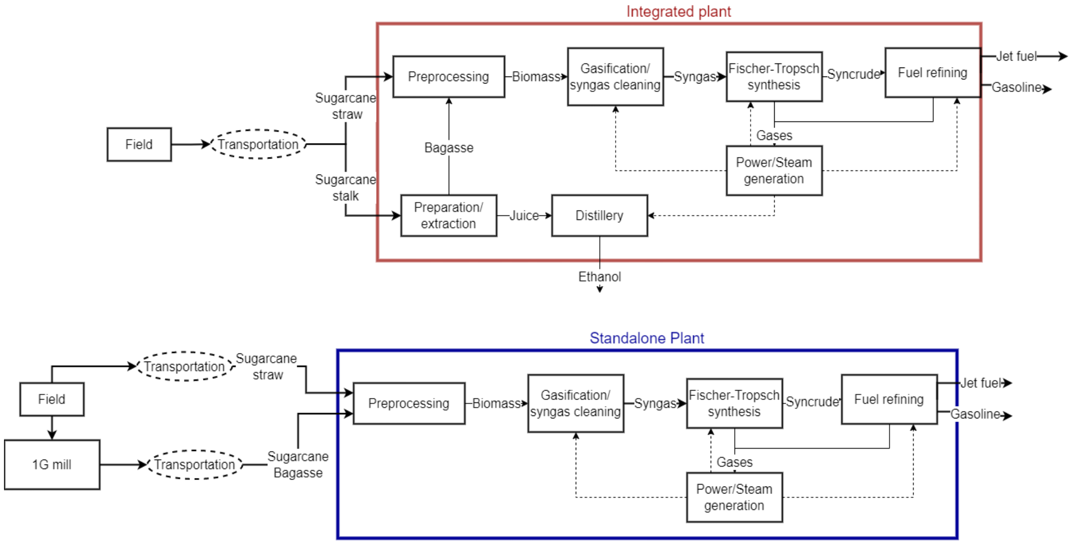

Figure IV-1 – Simplified process flowchart for the integrated and standalone configurations

The Virtual Biorefinery (VB) (Bonomi et al., 2016) was used as a tool to perform techno-economic and environmental analyses of both SA and INT scenarios. The VB is a software framework developed at the Brazilian Biorenewables National Laboratory (LNBR) from the Brazilian Center for Research in Energy and Materials (CNPEM), which allows the assessment of different biorefinery configurations. The agricultural phase was simulated with the CanaSoft® model, a part of the VB framework (Bonomi et al., 2016). An optimized scenario for sugarcane production was considered, with full mechanization of the agricultural stage and straw collection from the field. All agricultural operations were taken into account, from soil preparation to biomass transportation to the mill. The industrial phase of the biorefinery was simulated with the Aspen Plus® process simulator version 8.6 (AspenTech, Bedford, MA, USA). The simulation and its parameters are described in a previous study (Guimarães et al., 2021). For the economic evaluation of the scenarios, a discounted cash flow analysis was carried out considering a greenfield project. The main metrics adopted are the net present value (NPV), the internal rate of return (IRR), as well as the biofuel production costs.

The Life Cycle Assessment (LCA) tool was used to evaluate the environmental impacts of these scenarios, considering the use of the VB platform, which follows the methodology described by ISO 14000. The ecoinvent database provided the environmental profile of the background products and activities. For this analysis, economic allocation was used to account for the different outputs, and the use of resources and emissions for the whole production chain were included in the system boundaries, from biomass production to fuel use. Life cycle impact assessment were calculated for Climate Change impact category considering the 100-year time horizon global warming potential (GWP 100) from IPCC 2013. These results are used to calculate the avoided GHG emissions compared to fossil equivalent scenarios. Avoided GHG emissions are calculated from the difference between the biofuel and the corresponding fossil fuel – diesel, jet, and gasoline. These carbon intensities (gCO_2 eq MJ^{-1}) from the life cycle of fossil fuels were obtained from RenovaBio/RenovaCalc (ANP, n.d.).

The National Biofuels Policy (RenovaBio) is a policy already in motion in Brazil which imposes the distributors to prioritize the commercialization of a minimum required amount of biofuels via the generation of CBIO (Decarbonization Credit), a tradeable financial asset issued by the biofuel producer (de Souza, et al., 2018). This policy is considered in this study. With this in mind, an average price of 10 US$ per tonne of avoided CO_2 eq emission was considered (1 t of avoided CO_2 eq emission = 1CBio), although volatility in CBio prices have been observed over the last couple of years, with its value ranging from 3-20 US$ t^{-1} of avoided CO_2 eq (UNICA, n.d.).

3 - Results and Discussion

Table IV-1 presents the main results of both scenarios – standalone (SA) and integrated (INT). Overall, the integrated scenario presents better economic performance, with almost double the IRR of the standalone scenario. This trend is in line with that observed by Klein et al. (2018) and Bressanin et al. (2020) that the commercialization of ethanol can help increase the profitability of the plant. This can be seen for the total revenue, as the ethanol commercialization in the integrated plant more than doubles the revenue of the plant compared to the standalone BtL unit. This improvement also occurs because the production costs of the integrated configuration are 26% lower than those of the standalone configuration. This is mainly due to the influence of ethanol commercialization and, therefore, allocation of costs to this main product. The results of Table IV-1 also highlight the participation of the decarbonization credits in the total revenue of the plant. In terms of gross value, the annual revenue from CBios is in the range of 4 MUS$ in the standalone scenario and 9 MUS$ in the integrated configuration. This magnitude of revenue helps offset some of the costs, such as the mill inputs and labor expenses.

Table IV-1 – Main outputs and economic results

Results	SA	INT	Results	SA	INT
Total revenue (MUS$/year)			Total production costs		
Bioethanol	0	190	Bioethanol (US$/L)	-	0.43
Biojet fuel	62	49	Biojet fuel (US$/L)	0.71	0.52
Green gasoline	20	16	Green gasoline (US$/L)	0.62	0.45
Electricity	51	45	Electricity (US$/MWh)	71.83	52.58
Carbon credits	4	10	Total investment costs (MUS$)	609	740
Process outputs			Fixed capital investment (MUS$)	553	672
Bioethanol (ML/year)	0	440	Working capital (MUS$)	55	67
Biojet fuel (ML/year)	119	95	Annual operational costs	78	177
Green gasoline (ML/year)	45	35	Economic metrics		
Total GHG emissions	0.04	0.22	IRR (%/year)	5.9	11.9
Avoided emissions	0.36	1.02	NPV (MUS$)	-218	-7

Figure 2a presents the production costs breakdown of biojet fuel for both scenarios, and it is visible that the integrated plant corresponds to lower production costs than those from the standalone configuration. Figure IV-2a allows to better evaluate the influence of different factors on the economic feasibility. Capital expenditure (CAPEX) is the largest component of the production costs of the standalone configuration and almost half of the costs of the integrated scenario. The thermochemical route is very intensive in capital due to a large number of reactors and units for syngas cleaning and conditioning (Baliban et al., 2013). The 1G mill technology, however, represents a smaller percentage of the production costs, corresponding to only around 20% of the CAPEX of the integrated scenario. The technology for 1G ethanol production is considerably cheaper than the BtL technology, since second-generation (2G) thermochemical plants are more complex and expensive to build (Bressanin et al., 2020). To better exemplify the differences in technological maturity between 1G and 2G technologies, the 1G technology presents a ratio of 0.3 US$ of capital investment for each liter of fuel produced annually, while in the BtL route this ratio is in the range of 4 US$/L of fuels. Even though the data of Table 1 indicate that the integrated scenario presents higher investment costs than the standalone plant, when comparing the influence of these factor on the total production costs, the overall influence of the total CAPEX is less pronounced. This is due to the allocation of the total production costs along the different products, especially ethanol, which is the main product in the integrated case.

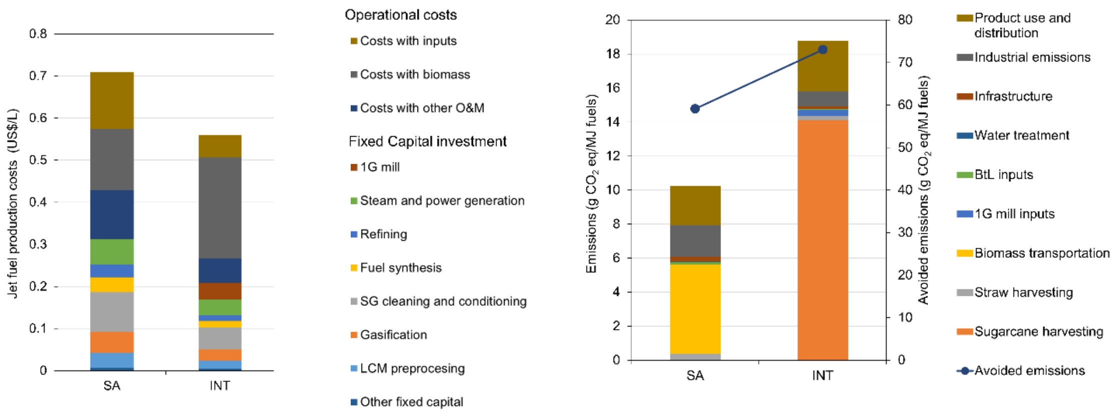

Figure IV-2 – (a) Biojet fuel production costs breakdown and (b) total emissions and avoided emissions (CO_2 eq)

In the case of operational expenditure (OPEX), a major contrast between both configurations is observed in terms of biomass acquisition. Many studies indicate that the expenses associated with feedstock can add up to almost half of the operational costs (Dimitriou et al., 2018; Holmgren et al., 2016) but, as can be seen in Figure IV-2, such value is below 20% for the standalone plant. This happens because biomass (sugarcane bagasse and straw) is cheaper than other biomasses (such as wood in other countries). For example, the wood prices are in the range of 50 US$/t on a dry basis (d.b.) (Dimitriou et al., 2018) or around 19-36 US$/MWh (Holmgren et al., 2016), while in the current study the LCM cost is in the range of 10-30 US$/t (d.b.) or 2-7 US$.MWh. This lower price leads to a lower participation of biomass costs in the overall production expenses, although sugarcane bagasse prices can vary considerably depending on the intensity of the dry season and the opportunity costs of electricity generation in the context of Brazilian mills.

As for the integrated configuration, higher biomass production costs are observed. The biomass for the standalone configuration is a mixture of bagasse and straw – both residues from sugarcane harvesting and 1G mill processing. As for the integrated plant, the biomass is the whole sugarcane from the fields, and thus the costs associated with cultivation and harvesting are directly linked to the costs of this biomass. This difference in biomass costs is aggravated due to the relatively high capacity of this configuration since that, in order to process 1 Mt dry LCM each year, the annual milling capacity of the integrated 1G mill is around 5 Mt of sugarcane. This means that the production costs of sugarcane – planting area, harvesting operations, and transportation costs – add up to a significant share of the total yearly OPEX. However, it is important to highlight that for Brazilian standards this is an achievable scale, since biomass availability is not a problem and nearly 10% of the sugarcane milling facilities have capacities of over 4 Mt of sugarcane per year (Conab, 2019).

Regarding other operational expenses, for both scenarios the high CAPEX of the BtL process results in high maintenance costs, while expenses on inputs for the thermochemical process are linked with high costs and catalyst consumption rates, especially those made from cobalt used in the FT process, whose price is in the range of 30-70 US$ per kg.

One important conclusion of this comparison is that, even with higher CAPEX and higher operational costs (as seen in Table 1), the integrated plant still presents better economic results thanks to the higher yearly biofuel output, mainly associated with 1G ethanol production. However, as pointed out in a previous study (Guimarães et al., 2021), the high electricity and heat consumptions of the 1G mill increases the demand for syngas diverted for steam and power generation. This results in a less energy-efficient process with lower production of biojet fuel and green gasoline in the integrated scenario. Since more syngas is recycled back to the FT reactor, the total investment of the fuel synthesis stage (FT reactor and syncrude refining) is larger in the standalone plant than in the integrated configuration. The opposite occurs in the steam and power generation unit. However, this difference has a limited effect on the overall investment cost of the BtL plant since the processes in both configurations have investment costs around 500 MUS$.

Figure 2b presents the breakdown of the GHG emissions of both scenarios. Overall, the integrated (INT) configuration presents higher total emissions, mostly due to the agricultural stage of the production chain. Sugarcane planting and harvesting are related to the consumption of fertilizers, pesticides, and fuels for machines. These categories have relatively high environmental impacts, thus increasing the overall carbon discharge. As for the standalone scenario (SA), bagasse is considered a residue from the 1G mill, thus presenting no impact directly associated with it. The straw collection is done in the form of bales, and it is associated with the necessary machines to collect this material, besides the allocation to it of some impacts from sugarcane harvesting. However, the overall impact of the straw collection is far less pronounced than the total impact of sugarcane. The main impact associated with biomass acquisition for the SA configuration is due to biomass transportation from the field and from the 1G mill to the BtL plant, and this section of the production chain corresponds to over half of the SA emissions. However, even though the INT scenario presents higher emissions, there are more avoided emissions compared to fossil fuel sources. This higher reduction is due to the production of 1G ethanol, which is a substitute for fossil gasoline in the Brazilian market.

4 - Conclusions

The present study points out the integration with a sugarcane mill is economically and environmentally beneficial to the BtL route. While a standalone plant was only able to obtain internal rates of return below 6%/year, the integrated configuration was able to achieve IRR between 10-12%/year. Also, the integration with a distillery increased 1.6 times the total avoided GHG emissions compared to the standalone BtL plant. The production of ethanol benefits both the direct revenue from fuels and the generation of decarbonization credits, further improving the revenue. Both standalone and integrated configurations can significantly reduce GHG emissions compared to fossil fuel sources and, consequently, the acquisition of carbon credits (CBios) is important to the revenue of both plants. However, it is possible to further reduce the environmental impacts. The standalone plant may focus on reducing emissions associated with biomass transportation by optimizing logistic aspects while also aiming at reducing costs with biomass acquisition. As for the integrated plant, biomass cultivation and harvesting demand some attention, both to reduce emissions (via substation of fossil diesel with green diesel) and operational costs. Overall, integration between thermochemical and biochemical routes has the potential to produce attractive economic results. Special attention should be given to mitigating the high costs with fixed capital, and biomass acquisition and transportation should also be the focus of a detailed evaluation. Incentives and policies are also important to the economic feasibility of the plant; however, some effort is required to fully assess the influence of carbon credits on the revenue of these biorefineries.

Nomenclature

1G – First generation
2G – Second generation
BtL – Biomass-to-Liquids
CAPEX – Capital expenditure
CBio – Decarbonization credits
CNPEM - Brazilian Center for Research in Energy and Materials
CO_2 eq – Equivalent carbon dioxide emission
d.b. – Dry basis
FT – Fischer-Tropsch synthesis

GFT – Gasification/Fischer-Tropsch synthesis
GHG – Greenhouse gases
GWP – Global warming potential
IRR – Internal rate of return
INT – Integrated configuration
LCA – Life cycle assessment
LCM – Lignocellulosic material
LNBR – Brazilian Biorenewables National Laboratory
NPV – Net present value
O&M – operation and maintenance
OPEX – Operational expenditure
RENOVABIO – National Biofuels Policy
SA – Standalone configuration
VB – Virtual Biorefinery

Acknowledgments

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Chapter V - Decentralization options

The final paper for this PhD project was submitted on the journal Energy Conversion and Management. This paper is still under evaluation from reviewers.

Decentralization of Sustainable Aviation Fuel production in Brazil through Biomass-to-Liquids routes: a techno-economic and environmental evaluation

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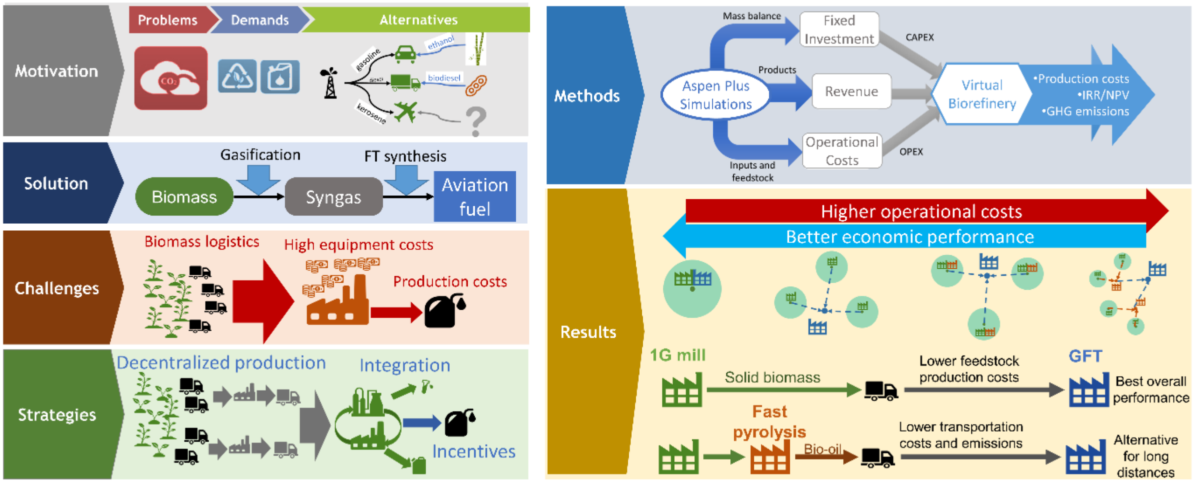
Abstract

The present study evaluated the influence of three strategies to improve the economic feasibility of sustainable aviation fuel (SAF) production through gasification and Fischer-Tropsch synthesis (GFT) of lignocellulosic biomass feedstocks in Biomass-to-Liquids (BtL) plants. Apart from the integration with sugarcane ethanol production and the use of economic incentives by the carbon credits market, we evaluated the decentralization of the production chain with fast pyrolysis (FP) units to densify the biomass into bio-oil, aiming to reduce feedstock transportation costs for biofuel production. These analysis made use of process simulation coupled with techno-economic assessment (TEA) and life cycle assessment (LCA).

Carbon credits commercialization alone is not enough to enable the standalone GFT scenario with current prices (up to 30 US$/tonne $CO_{2\ eq}$ avoided). However, integration into a 1G mill can decrease SAF production costs to as low as 0.4-0.7 US$/L and achieve over 70 g of $CO_{2\ eq}$ avoided/MJ of SAF. The addition of the FP process for decentralization is a better option than a centralized production only for distances above 1,000 km. This is due to expenses

with feedstock bio-oil being from 2 to 5 times higher than with the direct use of solid biomass. In conclusion, the path to make SAF production feasible lies in the integration with more mature routes and by relying on incentives from environmental policies, while the decentralization could help markets with highly disperse biomass availability.

Graphical abstract



Keywords:

Sustainable aviation fuel; sugarcane; Fischer-Tropsch; gasification; fast pyrolysis

Highlights

1. Different configurations for sustainable aviation fuel production were evaluated
2. Increasing carbon prices up to 140 US$/tonne enables the standalone GFT route
3. Integration can reduce production costs by 36% and avoid 160% more emissions
4. Decentralization with pyrolysis is viable only for distances above 1000 km

Nomenclature:

1G – First Generation

2G – Second generation

BtL – Biomass-to-Liquids

CAPEX – Capital expenditure

CBio – Decarbonization credits

$CO_{2\ eq}$ – Equivalent carbon dioxide emission
d.b. – Dry basis
FT – Fischer-Tropsch synthesis
FP – Fast pyrolysis
GFT – Gasification/Fischer-Tropsch synthesis
GHG – Greenhouse gases
GWP – Global warming potential
IRR – Internal rate of return
LCA – Life cycle assessment
LCM – Lignocellulosic material
NPV – Net present value
OPEX – Operational expenditure
RenovaBio – National Biofuels Policy
SAF – Sustainable aviation fuels
VB – Virtual Biorefinery
w.b. – wet basis

1 - Introduction

The increase in atmospheric CO_2 from 2019 to 2020 was higher than the average from the last decade despite the recent global crisis and restrictions caused by the COVID-19 pandemic. The last seven years (2015-2021) were the warmest years on record [1] and, therefore, we need to change the way we produce, transport, and consume energy to maintain the goal of net-zero emissions by 2050. However, according to the International Energy Agency (IEA) [2], the technologies and routes already available are not enough to achieve this goal. Thus, much of the necessary reductions will come from technologies that are still at the demonstration or prototype stage. This is the case for the aviation sector [2], whose liquid fuels demand is projected to continue growing [3]. This scenario is aggravated by the scarcity of readily available fuel options to achieve carbon emissions neutrality by 2050. To achieve this goal, it is expected that at least 50% of the fuel used in aviation by 2040 should be clean [2].

Although there are currently approved routes to produce low-emission Sustainable Aviation Fuel (SAF), the most mature option - the Hydroprocessing of Esters and Fatty Acids

(HEFA) – is not enough to supply the demand for SAF entirely [4]. Among the alternatives, the thermochemical Biomass-to-Liquids (BtL) path appears as a promising option [5]. The BtL pathway is particularly interesting thanks to the possibility of processing different kinds of feedstocks into a wide range of fuels [6]. This process usually is comprised of the gasification of biomass, followed by Fischer-Tropsch (FT) synthesis to produce liquid fuels such as SAF, green diesel, and green gasoline. These fuels present similar characteristics to fossil fuels with the added benefit of lower emissions [7]. However, many airline companies are reluctant to incorporate SAF due to higher operational costs [5]. Large-scale implementation of gasification and FT conversion (GFT) processes is also hindered by high equipment costs [8] and the cost gap between fossil-based and biobased fuels [9]. As a consequence, many of the existing GFT plants are still at the demonstration stage [10].

Despite these setbacks, the key to achieving net zero emissions may lie in improving BtL technologies on a commercial scale [2]. In this sense, the creation of policies and government aid could help improve the competitiveness of biofuels. For instance, the ReFuelEU aviation initiative aims to enhance the uptake of SAF in Europe by enforcing fuel suppliers to distribute these fuels at European Union airports [11]. Another example is the Brazilian National Biofuels Policy (RenovaBio), which has created a market of carbon credits to incentivize fuel producers and distributors to adhere to biofuels, which will contribute to mitigating emissions from road to aviation transport sectors [12,13].

Besides governmental aid, other measures can push the implementation of advanced biofuel production routes in the Brazilian context. In their study, Bressanin et al. [14] point out that the BtL route can benefit from integration with First-generation (1G) ethanol production process. The revenue from ethanol commercialization lowers the risk associated with high investment and operational costs. This observation was confirmed in another work [15] that found that the integration into a 1G mill could achieve the minimum internal rate of return required for this type of investment (at least 12% per year).

Increasing the nameplate capacity of BtL plants improves their feasibility, but the gains from scaling up are limited due to increased feedstock costs and longer transportation distances [16]. However, these setbacks can be overcome by improving biomass productivity with different harvesting technologies, densifying the biomass to lower transportation costs, and using transportation with different logistics configurations [17]. Lower-scale decentralized units can be implemented near feedstock production sites, inducing lower costs in feedstock transportation and handling for this production chain [18].

The use of fast pyrolysis (FP) as a biomass densification method could be advantageous since bio-oil is an intermediate of higher energy density than biomass, which could reduce transportation costs [19]. Unlike gasification and FT plants, FP units can be economically viable on relatively smaller scales [20], thus being well suited for this application.

The present work aims at evaluating the production of SAF through the GFT route, by considering the main possible implementation strategies in the Brazilian sugarcane industry. This study highlights the influence of the existing sugarcane infrastructure along with an ongoing incentive policy (RenovaBio) based on the greenhouse gas (GHG) intensity performance of the biofuel produced. The novelty of the present paper comes from considering the integration of the main route – gasification/FT conversion and the Brazilian sugarcane sector based on biochemical platforms – with the implementation of pyrolytic units for biomass densification as a way to improve economic and environmental performance. The goal is to assess these different strategies both in terms of economic and environmental performance (through techno-economic analysis – TEA, and life cycle assessment – LCA, respectively). The integration, decentralization, and the use of incentive policies are evaluated to increase SAF feasibility. Thus, this study may assist the global effort of pinpointing more sustainable solutions and verifying scenarios in which BtL biofuels could compete and substitute fossil aviation kerosene.

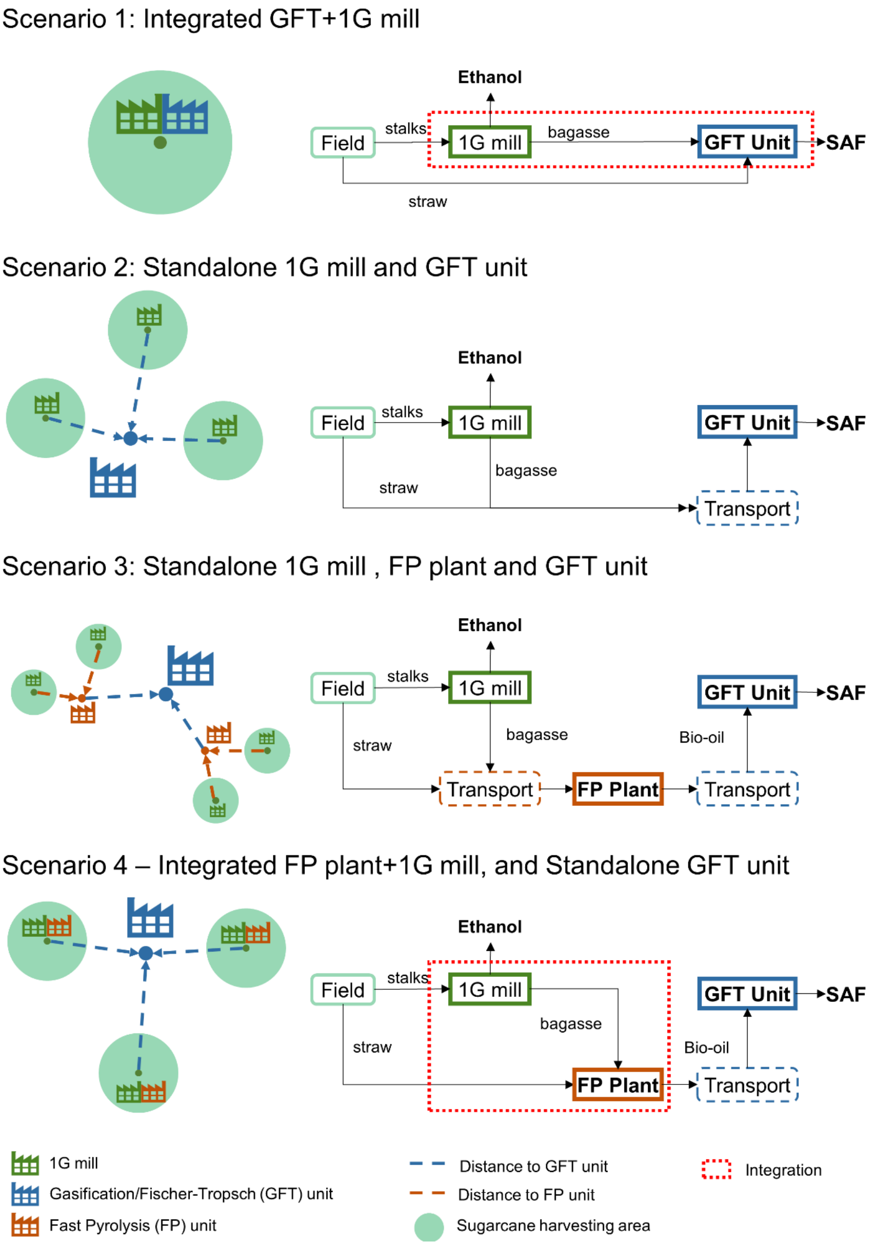
2 - Methods

2.1. Scenarios Description

The first configuration for SAF production consists of a GFT plant integrated into a first-generation ethanol distillery (1G mill). This scenario, called “Scenario 1”, was presented in a previous study [10]. The sugarcane mill operates during the sugarcane season (200 days/year) processing biomass to obtain hydrous ethanol through fermentation of sugars. The straw collected on the field and the bagasse produced during the juice extraction are directed to an integrated thermochemical plant that operates 330 days per year. In the thermochemical plant, this lignocellulosic material (LCM) is gasified and converted into SAF by FT synthesis.

The second configuration ("Scenario 2") is a standalone BtL unit operating 330 days/year by purchasing and stocking LCM from nearby 1G mills. This scenario is considered the "centralized" case, where a single GFT unit receives all the required LCM from mills surrounding the plant.

It is also possible to account for FP units, which densify the LCM into bio-oil and supply it to a GFT unit to be gasified and converted into SAF. This configuration corresponds to the decentralization of the SAF production chain. The 1G mills supply the FP unit with LCM, while the FP plants supply the GFT process with bio-oil as a feedstock. There are two possible alternatives for these FP units. The first considers standalone FP plants purchasing LCM from nearby 1G mills (Scenario 3). The other possibility is for these FP units to be integrated into 1G mills (Scenario 4). Figure V-1 presents a summary of the considerations for each case along with an overview of the distribution of the units for each scenario, and a simplified flowchart of the processes.



Scenario 1: Integrated GFT+1G mill

Scenario 2: Standalone 1G mill and GFT unit

Scenario 3: Standalone 1G mill , FP plant and GFT unit

Scenario 4 – Integrated FP plant+1G mill, and Standalone GFT unit

Figure V-1 – Overview of the spatial configuration of each scenario, and the simplified flowchart for the production chain

2.2.Feedstock acquisition options

The proposed scenarios are dependent on three "feedstocks": the sugarcane supplied to the 1G mill; the LCM supplied to the GFT unit or the FP unit; and finally, the bio-oil supplied to the GFT plant.

(1) Sugarcane harvesting (integrated scenarios)

The simulation of sugarcane production was performed using the CanaSoft model, a platform developed as part of the Virtual Biorefinery (VB) framework [21]. CanaSoft comprises all agricultural operations (from soil preparation to biomass transportation to the mill), considering a variety of inputs such as machinery, implements, trucks, and labor. The scenarios considered the optimal and current configuration available for new sugarcane biorefineries, and the full mechanization of the agricultural stage. Table S.1, in the Supplementary Material, presents the considerations for the agricultural stage.

(2) First-generation ethanol distillery (integrated scenarios)

The operational parameters for the industrial stage of the 1G mill were obtained from the literature [22], considering an optimized autonomous ethanol distillery as the basis for integration with the thermochemical plant. Further detailing of this modernized distillery is available in the Supplementary Material (Figure S.1 and Table S.2) and the literature [23,24]. This 1G mill operates during the sugarcane season (200 days/year) with a total processing capacity of 4 million tonnes of sugarcane/year, producing hydrous ethanol.

(3) LCM acquisition

The demand for LCM is assumed to be supplied by the sugarcane sector in the form of sugarcane bagasse and straw. There is currently no established market for bagasse since most of this material is burned inside the mills to generate electricity. Nonetheless, this study assumed a developed market for sugarcane bagasse, following the prices proposed in the works from SUCRE (Sugarcane Renewable Electricity) project in Brazil [25]. For the production and supply of sugarcane straw, not all straw produced can be harvested, since a remaining fraction must be left on the field to help maintain soil quality [25]. Thus, the process collects only 50% of the available sugarcane straw on the field in a second-pass straw harvesting operation. The costs and environmental impacts of the straw collection are calculated using the CanaSoft model [21].

(4) Bio-oil production by FP of solid biomass

Since bio-oil does not have yet an established market, its selling price – or levelized production cost – was calculated for each configuration to achieve a desired internal rate of return (IRR). For all scenarios involving bio-oil production, the perspective of a project belonging to the sugarcane industry was assumed. In the standalone plant, this unit does not have a direct alternative or competitor, so a minimum acceptable rate of return of 12% per year was considered [21]. The integrated configuration, however, competes with an existing 1G mill, so the minimum selling price of bio-oil was set to match the IRR of a similar standalone 1G ethanol distillery.

The simulation of the FP process was performed using the software Aspen Plus (V 9.0) through a kinetic approach based on the works of Ranzi et al. [26] and Salina et al. [27]. The biomass is first ground and dried to a moisture content of 5 wt%. The fluidized bed pyrolysis reactor operates with a temperature of 475 °C and pressure of 1.5 bar, with a flow of nitrogen gas to ensure an inert atmosphere. The bio-oil from the outlet stream of the reactor is recovered, and the non-condensable gases are burned together with the char to generate the heat and electric energy required for the process. The exhaust gases from the burner are used to provide the thermal energy necessary for both the reactor and the fluidizing gas (nitrogen). For the standalone FP configuration, no additional production of steam and heat is necessary; thus, the remaining energy generation from the burner is used to generate electricity through a Rankine cycle. For the integrated configuration, the 1G mill represents an extra energy demand for steam, so the energy and heat generation on the plant is changed to a combined cycle processing the gases to produce both electricity and utility steam.

Section S.II.a of the Supplementary Material presents a detailed description of the FP process.

2.3.SAF production

The specific process design of the GFT stage depends on the scenario type (see Figure V-1), with all scenarios conceived to be energy self-sufficient.

The configuration for Scenario 1 follows the description given in our previous study [10]. After the 1G mill process, bagasse and straw are stored to supply LCM to the thermochemical plant during the sugarcane season and off-season operations. The gasification process operates in a low-pressure indirectly-heated circulating fluidized bed gasifier with superheated steam (310 °C and 2.5 bar) as a gasifying agent at a ratio of 0.4 $\text{tonne}_{\text{steam}}/\text{tonne}_{\text{dry LCM}}$. The syngas cleaning stage for Scenario 1 consists of tar reforming, cooling/quenching, acid gas removal (AGR), pressurization, and pressure swing adsorption (PSA). The FT synthesis is performed in a tubular fixed bed reactor with cobalt catalyst at 25 bar and 200 °C. The products are separated in a gas/liquid knock-out separator, and the liquids are directed to a refinery section developed to maximize the production of SAF with the co-production of green gasoline, following a design proposed by Klerk [28]. This configuration was chosen since the main focus of this project is the production of jet fuel. A fraction of the gases is recycled to the reactor, while the remaining is diverted to generate heat for the catalyst regenerator (tar reforming) and to a gas turbine for power and steam generation [29]. Different process integrations were assumed to ensure the generation of heat and steam required in the process. The Supplementary Material contains a more detailed description of the considerations for the process and simulation of Scenario 1, besides information pertinent to costs and investment estimates.

Scenario 2 has the same configuration for the thermochemical process as Scenario 1, but with lower steam and electricity demands. This difference in Scenario 2 means that a larger fraction of the unreacted gases can be recycled to the FT reactor. In Scenario 1, 40% of the syngas is recycled, while in Scenario 2, over 80% of the gases can be recycled back to the FT reactor. This difference in recycle ratios leads to higher liquid fuel yields for the standalone Scenario 2 than for the integrated Scenario 1, as shown in previous studies [15,30].

Different GFT process designs were considered for Scenarios 3 and 4. First, the gasification process occurs in a pressurized entrained-flow reactor, operating at 1200 °C and 25 bar with pure oxygen as the gasifying agent (Equivalence ratio = 0.3). The outlet stream is cooled to 500 °C. Around 2% of the inlet mass is converted into soot [31], which is then separated and burned. The syngas from bio-oil gasification has lower methane and tar contents, and the operational conditions of the reactor favor water-gas shift reactions. With these considerations, the cleaning stage of the bio-oil-based syngas is composed only of a cooling stage with contact with water (coupled to the outlet of the reactor), an AGR unit, and the PSA process. The FT synthesis, refining, and combined cycle for energy production are similar to Scenarios 1 and 2. Sections S.II.b to S.II.d in the Supplementary Material detail the simulation and considerations of the GFT process.

2.4.Transportation costs and GHG emissions calculation

The impacts of transporting feedstocks and products were calculated based on the VB framework. This tool allowed us to determine both the LCM and bio-oil transportation costs for each scenario, as well as the life-cycle GHG emissions for each case.

A hypothetical scenario first considered the supply of biomass to be obtained from sugarcane fields and 1G mills of similar capacities and selling 100% of the available LCM. By fixing the capacity of the BtL plants, it is possible to determine the number of required biomass-supply units. Given the number of necessary suppliers, we calculated the hypothetical minimum distance necessary to transport the material with the following considerations:

- Each biomass-supply unit is placed at the minimum distance possible from the others;
- Every 1G mill and its respective sugarcane crop supplying bagasse/straw/sugarcane have the same size;
- The harvesting area (determined by the radius) of each 1G mill does not overlap with that of other mills;
- BtL plants are equidistant from the biomass-supply units.

The spatial distribution of these different units takes into account that the BtL plants are in a central position. The different suppliers are then distributed uniformly and equidistantly to the central BtL plant, thus allowing the calculation of the average distance of transportation of the LCM and bio-oil. This theoretical configuration provides a standardized location setup that isolates the effects of varying the total transport distance on the techno-economic and environmental impacts of the different scenarios. Further explanation of these calculations can be found in the Supplementary Material (Section S.III).

2.5.Life Cycle Assessment

The present study uses the Life Cycle Assessment (LCA) as a tool to evaluate the environmental impacts of each scenario. The LCA follows the methodology described by ISO 14000 [32,33], integrating the foreground inventories (biomass production, transport, and conversion to biofuels) modeled according to the VB framework. The ecoinvent database [34] describes the background inventories for products and activities involved in the production of SAF. For this analysis, energy allocation determined the share of impacts between the different outputs. The system boundaries include the use of resources and emissions for the whole production chain, from biomass production to fuel use. This study focused on Climate Change as the main environmental impact category considering the 100-year time horizon global warming potential (GWP 100) from IPCC 2013 [35]. Section S.IV in Supplementary Material presents the different inventories for each process considered. The estimation of the inventory considers that much of the GHG emissions associated with biomass processing are biogenic and have zero impact, since they are compensated by the carbon uptake from the photosynthesis of sugarcane.

The results from the environmental analysis allowed the estimation of avoided GHG emissions, in comparison to fossil-equivalent scenarios. The difference between biofuel and its equivalent fossil fuel results in the Avoided GHG emissions. The benchmark carbon intensities (g $CO_{2\ eq}$/MJ) from the life cycle of fossil fuels followed the standard values from RenovaBio/RenovaCalc [13] (87.5 and 87.4 g $CO_{2\ eq}$/MJ for fossil jet fuel and gasoline, respectively). According to the avoided emissions, a given quantity of carbon credits was issued as revenue for the plant, based on 1 tonne of avoided $CO_{2\ eq}$ = 1 CBio. The prices of the CBios are market-dependent since they are traded in the Brazilian stock market, with an average price of 10 US$/tonne of avoided $CO_{2\ eq}$ per year [36]. A sensitivity analysis was performed for Scenarios 1 to 4 to verify the influence of the variations in historical prices of CBios since the implementation of Renovabio [36].

2.6.Techno-economic analysis

The main inputs necessary to carry out the techno-economic analysis are the investment, operational costs, and the project revenue. The CAPEX (capital expenditures) was calculated based on the available VB database (which has a detailed description of equipment and engineering costs associated with the construction of sugarcane mills) as well as data on equipment for thermochemical conversion were taken from Dutta et al. [37], Swanson et al. [38], and Nexant [39] for the LCM GFT; Tijmensen et al. [40] for FT synthesis; Wright et al. [41] for the LCM FP; and Trippe et al. [42] and Neves [43] for bio-oil GFT. The annual OPEX (operational expenditures) was estimated by calculating the costs of different feedstocks, chemical inputs (enzymes, reactants), maintenance, labor, and catalyst prices, among other components. This study considered the standardization of all costs to December 2019 US$, and the Supplementary Material (Section S.V) presents all the considerations for the TEA.

The main prices of products – gasoline and SAF – were estimated based on the ten-year average historic data available in the Agência Nacional de Petróleo, Gás Natural e Biocombustíveis database [44] to quantify the revenues from the different scenarios. Based on the discounted cash flow analysis, the production cost, internal rate of return (IRR), and net present value (NPV) [45] of the different scenarios were calculated to select the most competitive alternatives.

2.7.Uncertainty analysis

This study performed an uncertainty analysis to analyze the impact of the many variables considered in this study both on the economic and environmental outputs from the models. In our previous study, the main factors to influence the economic feasibility of the BtL route were identified. These included products (fuels and electricity); capital investment; inputs costs (catalysts and other chemicals); and feedstock cost [10]. This analysis considered the historic variation of the prices and costs of these factors, which were obtained from the historical data from the market over the past 10 years. The variation for the CAPEX was associated with the uncertainties and accuracy of the estimation of the total capital cost, ranging from -10% to +30% [46]. The SUCRE project report [25] provided the costs of sugarcane bagasse. Sugarcane yield is the main parameter associated with the production of sugarcane and straw. This parameter has a direct influence both on the energy and cost intensity of biomass production, as well as on the transportation distance which, in turn, is an important driver of the environmental impacts of biofuel production. The final parameter chosen was the price of the CBios, whose volatility is an exogenous variable fully dependent on market conditions. For this parameter, we considered data from the previous two years (2020-2021). This range refers to the entire period of CBio trade since the RenovaBio policy has been established [13].

The risk assessment followed the Monte Carlo methodology. This methodology consists of a series of computational techniques for the approximate solution of mathematical problems, which make use of random samples to provide estimates of deterministic quantities [47]. The mathematical models were obtained from electronic spreadsheets (Microsoft Excel 2013) integrated with the industrial simulations (Aspen Plus V 8.0). These models were subjected to 10,000 runs using input values for the variables selected from multi-value probability distributions. The software XLRisk V 1.00 assisted this process, and each parameter (Table III-7) varied according to a triangular distribution. For each variable, the deterministic value was the most likely value, and the minimum and maximum values were determined by the relative range in Table III-7. These simulations resulted in a series of values for the main metrics of this study (NPV, IRR, GHG emission, production costs, and revenue). Thus, the uncertainty analysis provides the probability distribution of the potential outcomes for the different scenarios.

Table V-1 – Possible variation range for each parameter in the scenario analysis, considering triangular distributions.

	Deterministic value	**Min-Max.**	**Period**	**Source**
Gasoline price	0.45 US$/L	95-106%	2002-2019	[44]
Sugarcane yield	80 tonnes/ha	86-108%	2008-2019	[48]
Sugarcane bagasse cost	10 US$/tonne	40-210%	-	[25]
Ethanol price	0.43 US$/L	71-133%	2004-2019	[49]
Jet fuel price	0.53 US$/L	84-115%	2002-2019	[44]
Electricity price	54 US$/MWh	87-127%	2003-2019	[50,51]
CAPEX FP	Calculated	90-130%	-	[46]
CAPEX GFT	Calculated	90-130%	-	[46]
CAPEX 1G mill	Calculated	90-130%	-	[46]
Inputs costs	Calculated	37-106%	2009-2019	[52]

CBios price	10 US$/tonne avoided CO_{2eq}	37-250%	2020-2021	[53]

3 - Results and discussion

3.1. Feedstock production

The CanaSoft model allowed us to calculate the production costs and emissions associated with the harvesting of sugarcane stalks and straw. Figure V-2 presents these results and the range of values associated with the variation of the sugarcane yield (as described in section 2.7). These results are only related to the production/harvesting, disregarding the transportation of these materials. The costs and impacts of transporting these biomass materials are calculated on the evaluation of each scenario (sections 3.2 and 3.3).

According to Figure V-2.a, straw is more expensive than sugarcane stalks in terms of mass, particularly due to the lower density of straw compared to sugarcane. However, as shown in Figure V-2.b, the relative cost of straw is then significantly lower than that of stalks in terms of energy content (lower heating value – LHV). The cost for bagasse (not presented in Figure V-2) obtained from the literature [25] is in the range of 4-21 US$/tonne$_{\text{wet basis}}$. As a comparison., usual values for straw prices are in the range of 27-37 US$/tonne [54], 30-50 US$/tonne [25], or 20-40 US$/tonne [22]. The values for straw shown in Figure V-2.a are in the range observed in the literature. Bagasse price, however, is considerably cheaper than straw.

In terms of GHG emissions, both Figure V-2.c and 2.d show that the emissions allocated to the straw are one order of magnitude lower than the emissions of the whole sugarcane plant. This difference is mainly due to the allocation of the emissions from harvesting since the stalks represent the larger share of mass, energy, and revenue. According to the methodology from RenovaBio based on directives from the EU parliament [55], agricultural residues such as bagasse are considered to have zero life cycle GHG emissions – which have been followed in this study.

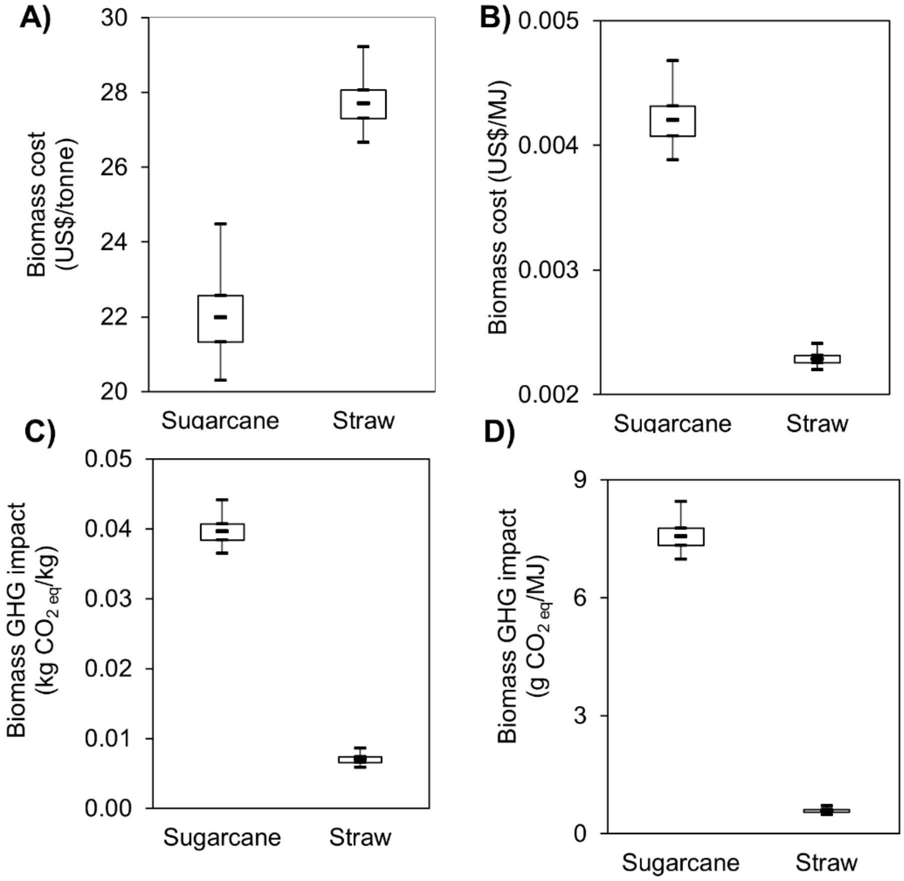


Figure V-2 – Production costs and total emissions of biomass production (wet basis): biomass production costs in (a) US$/tonne and (b) US$/MJ; associated GHG emissions in (c) kg $CO_{2\ eq}$*/kg and(d) kg* $CO_{2\ eq}$*/MJ.*

Figure V-3 presents the influence of scale on the production costs and minimum selling price of the bio-oil to assess the capacity of the FP units. From these results, the standalone configurations benefit from the increase in scale. Since bio-oil selling price is calculated as the required value to achieve an IRR of 12% per year (NPV = 0), the minimum selling price and the production costs are equal in the standalone scenarios. For capacities above 0.5 Mtonne of bio-oil per year, the decrease in bio-oil price is less pronounced, reaching an average price of 100 US$/tonne of bio-oil.

However, the integrated scenario (dashed lines in Figure V-3) has an increase in both bio-oil production costs and minimum selling price for higher capacities. This occurs because integrated configuration is set to follow the performance of a standalone 1G mill. The 1G mill benefits largely from increased scales up to 4-6 Mtonnes of sugarcane per year [56], corresponding to a capacity of around 0.4 to 0.6 Mtonne bio-oil/year. The commercialization of bio-oil offsets the higher investments and operational costs resulting from the integration with the thermochemical plant. This also explains the difference between the production costs and the minimum selling price of bio-oil for the integrated scenario.

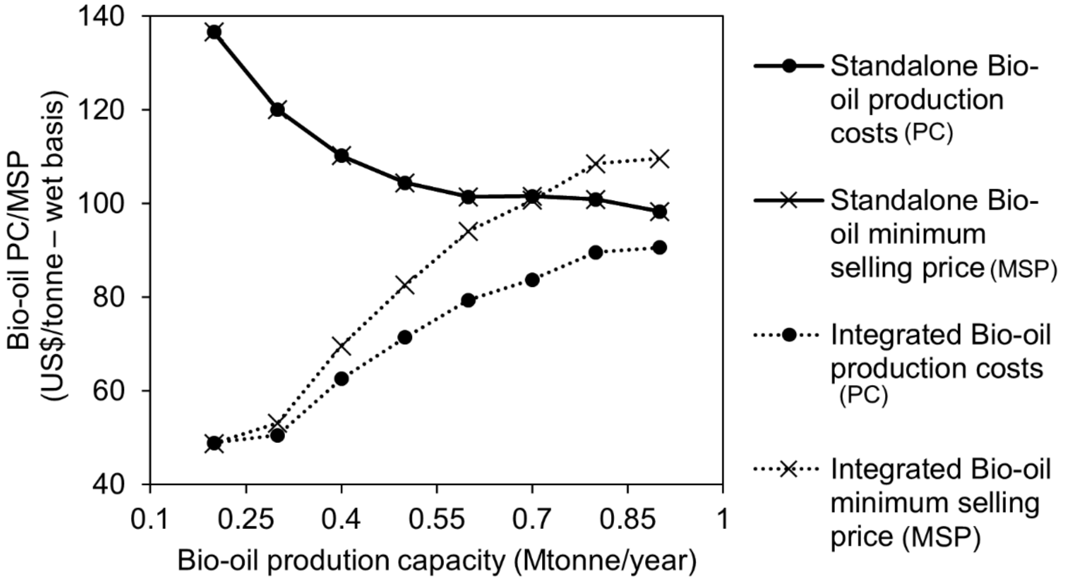


Figure V-3 – Influence of scale on the production costs and minimum selling prices of bio-oil in standalone (Scenario 3) and integrated (Scenario 4) scenarios.

These results indicate that the standalone FP unit is the most benefited from economies of scale. This influence is less pronounced for larger scales, and the fact that the average bio-oil price stays in the range of 100 US$/tonne. The relatively low reduction in costs for higher capacities indicates that there is some flexibility in choosing the operational capacity of the plant. Since the goal is to consider these units operating as decentralized densification units, the present study fixed the scale of the FP unit at the lower range below 0.6 Mtonne/year. The capacity set for the FP units was chosen as the production of the FP integrated into a 1G mill processing 4 Mtonnes of sugarcane per year, since this corresponds to a sufficient decrease in bio-oil production costs while maintaining the capacity compact enough for a decentralized unit.

Table V-2 and Figure V-4 present the main results of the two configurations for the FP densification units: standalone unit (Scenario 3) and integration into a 1G ethanol distillery (Scenario 4). Both configurations are set to operate at the same capacity (0.42 Mtonnes of bio-oil/year). The definition of the standalone scenario restricts the bio-oil minimum selling price to always achieve NPV = 0 (as explained in Section (4)). Thus, there is no variation related to the risk analysis on both NPV and IRR since these parameters are always set to 0 MUS$ and 12% per year respectively for these particular scenarios.

Table V-2 – Main economic and environmental results for bio-oil production through FP.

	Standalone (Scenario 3)	**Integrated (Scenario 4)**
NPV *(MUS$)*	0.00 (0 – 0)	87.62 (0 – 404)
IRR *(% per year)*	12 (12 –12)	16 (12 – 27)
NPV/CAPEX *(-)*	0.00 (0 – 0)	0.32 (0 – 1.37)
Capacity *(Mtonnes $_{LCM\ d.b}$/year)*	0.73	0.73
	-	4.00
Bio-oil production *(Mtonnes/year)*	0.42	0.42
Revenue *(MUS$/year)*	79.74 (65 – 98)	198.15 (164 – 282)
Total emissions *(Mtonnes$_{CO2\ eq}$/year)*	0.049 (0.048 – 0.049)	0.23 (0.22 – 0.25)

*SC: sugarcane

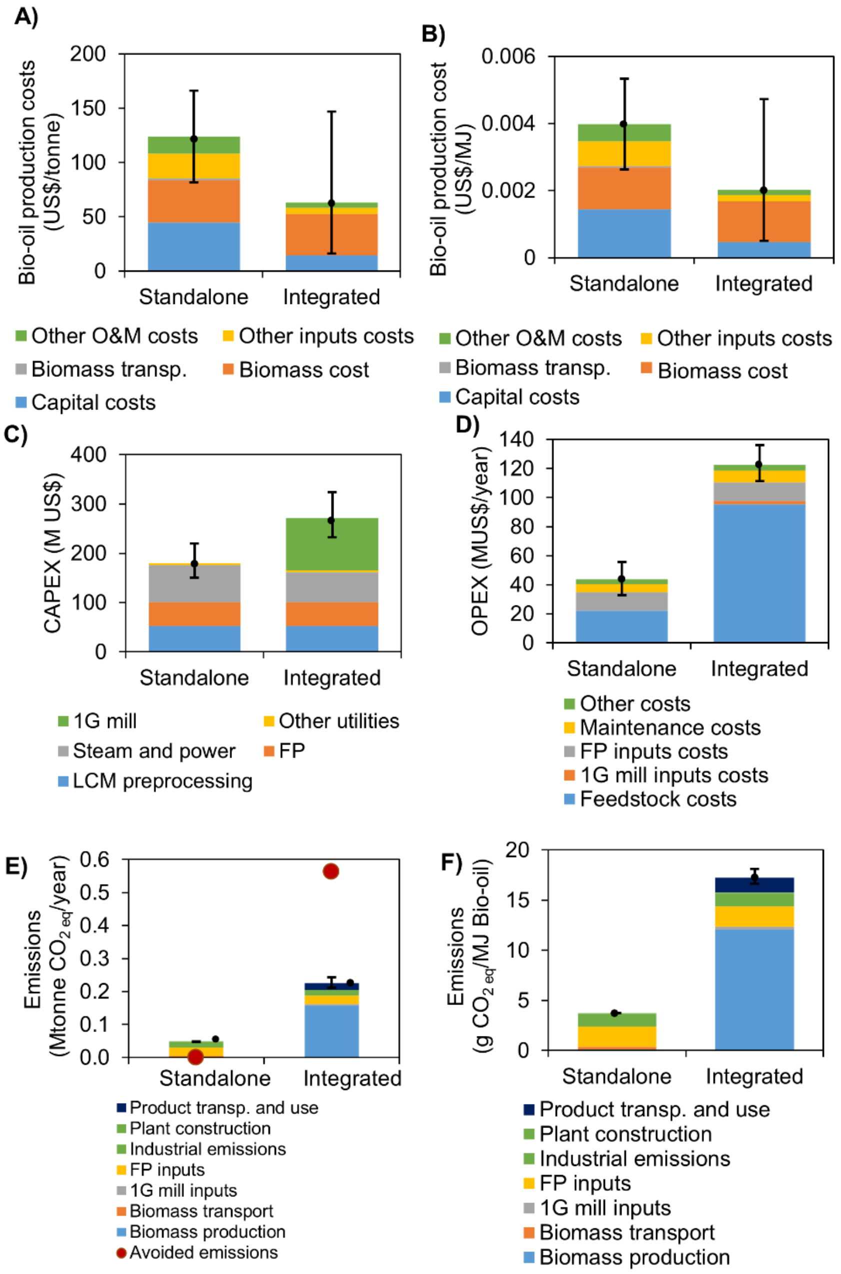


Figure V-4 – Economic and environmental results for FP of LCM in standalone (Scenario 3) and integrated (Scenario 4) scenarios: bio-oil production costs in (a) US$/tonne wet basis and (b) US$/MJ); (c) total investment breakdown (MUS$); (d) annual operational costs breakdown (MUS$/year); (e) total annual emissions (Mtonnes $CO_{2\ eq}$/year) ; (f) total emissions (g $CO_{2\ eq}$/MJ of bio-oil).

The difference in configuration also reflects on the CAPEX. For example, the configuration studied by Wright et al. [41] considers the hydroprocessing of the bio-oil. The addition of this step may correspond to an increase of at least 15-40% in investment costs. However, when comparing only similar processes (biomass preprocessing, pyrolysis, and utilities), the present study presents investment costs around 30% higher than those observed by Wright et al. The higher investment is attributed to the localization of the technologies to the Brazilian market [10], which increases the expenses to import and develop the different equipment.

Between the standalone and integrated configurations, differences in CAPEX and OPEX (Figure V-4.c and Figure V-4.d) are mainly associated with the operation of the 1G mill. The cost associated with the equipment of the mill is responsible for the higher CAPEX of the integrated scenario. The expenses with sugarcane and other mill inputs also lead to higher operational costs.

The bio-oil production costs are in the range of 0.09-0.18 US$/L for the standalone case, and 0.03-0.17 US$/L for the integrated scenario (Figure V-4.a). These values are below the production costs observed in the literature, within the range of 0.47 – 1.13 US$/L [57]. The main difference is that many of these works consider different configurations with bio-oil processing and upgrading, as well as more expensive biomass sources, as sugarcane bagasse and straw are relatively cheap, especially when compared with woody feedstocks [10]. For example, the evaluation by Vasalos et al. [58] assumed a biomass cost of 57 US$/ton d.b, a price almost twice the value for sugarcane and straw (Figure V-2.a). For the work from Li et al. [59], the proposed process includes stabilization and upgrading of the bio-oil, including consumption of natural gas, thus raising the costs of production if compared to the present results. Since the proposed configuration only considers the bio-oil as an intermediate energy carrier with little processing and upgrading, its overall production cost is relatively lower than those observed in the literature.

Despite the requirement of matching the economic performance of a 1G mill plant, the integrated scenario presents lower bio-oil production costs in comparison with the standalone unit (Figure V-4.a and Figure V-4b). The increased revenue from ethanol (Table V-2) is enough to offset the higher CAPEX and OPEX (Figure V-4.c and Figure V-4d) of the integrated configuration. According to Rahman et al. [18], the revenue gained from the commercialization of coproducts obtained from integration with other routes can reduce considerably the production costs of bio-oil and biofuels, given that the market is mature enough to absorb this production. This is easily the case for bioethanol in the Brazilian market since over 90% of the light vehicle fleet can operate either with gasoline or ethanol (or any mix of both) [60].

Another advantage of the integrated scenario is the revenue from carbon credits. This configuration counts with the commercialization of CBios from the avoided emissions in the production of ethanol (Figure V-4.e). The standalone scenario, however, cannot participate in the carbon credits market since its products (bio-oil and electricity) are not yet directly accounted for in the RenovaBio policy.

Still on the topic of environmental performance, from Figure V-4.e and Figure V-4.f, the margin of variation for the total emissions for both scenarios is narrow. The small range of variation is a consequence of only one parameter from the risk analysis being directly associated with emissions (Table III-7, Section 2.7) – the sugarcane yield. The only other factor that influences environmental performance is the distance of transportation of feedstock and products, which is further evaluated in this paper (Section 3.3).

Comparing bio-oil and biomass production costs on a mass basis, bio-oil (Figure V-2.a) assumes average values of 60 and 120 US$/tonne in the integrated and standalone scenarios, respectively. Thus, bio-oil is considerably more expensive than raw biomass (sugarcane and straw), which had average costs of 22-28 US$/tonne in Figure V-4.a. By considering an energy basis, however, bio-oil and biomass are in the same order of magnitude (Figure V-2.b and Figure V-4.b, respectively). Although FP can densify the feedstock, it nonetheless increases the final costs of SAF by embedding the additional costs of upstream processes into the SAF production chain. These additional steps also contribute to relatively higher emissions (Figure V-2.d and Figure V-4.f) and higher uncertainties (as seen by the wider variation margins) in scenarios using decentralized configurations.

3.2.SAF production

Figure V-5 and Figure V-6 present the main economic and environmental results for each SAF production scenario. All the scenarios are compared for the same production capacity of advanced fuels (SAF and green gasoline, with a total of 3.8 10^9 MJ of liquid fuel/year). The capacity is fixed based on the production of Scenario 1 (the base case scenario from our previous study [10], for an integrated plant processing 4 Mtonnes of sugarcane/year).

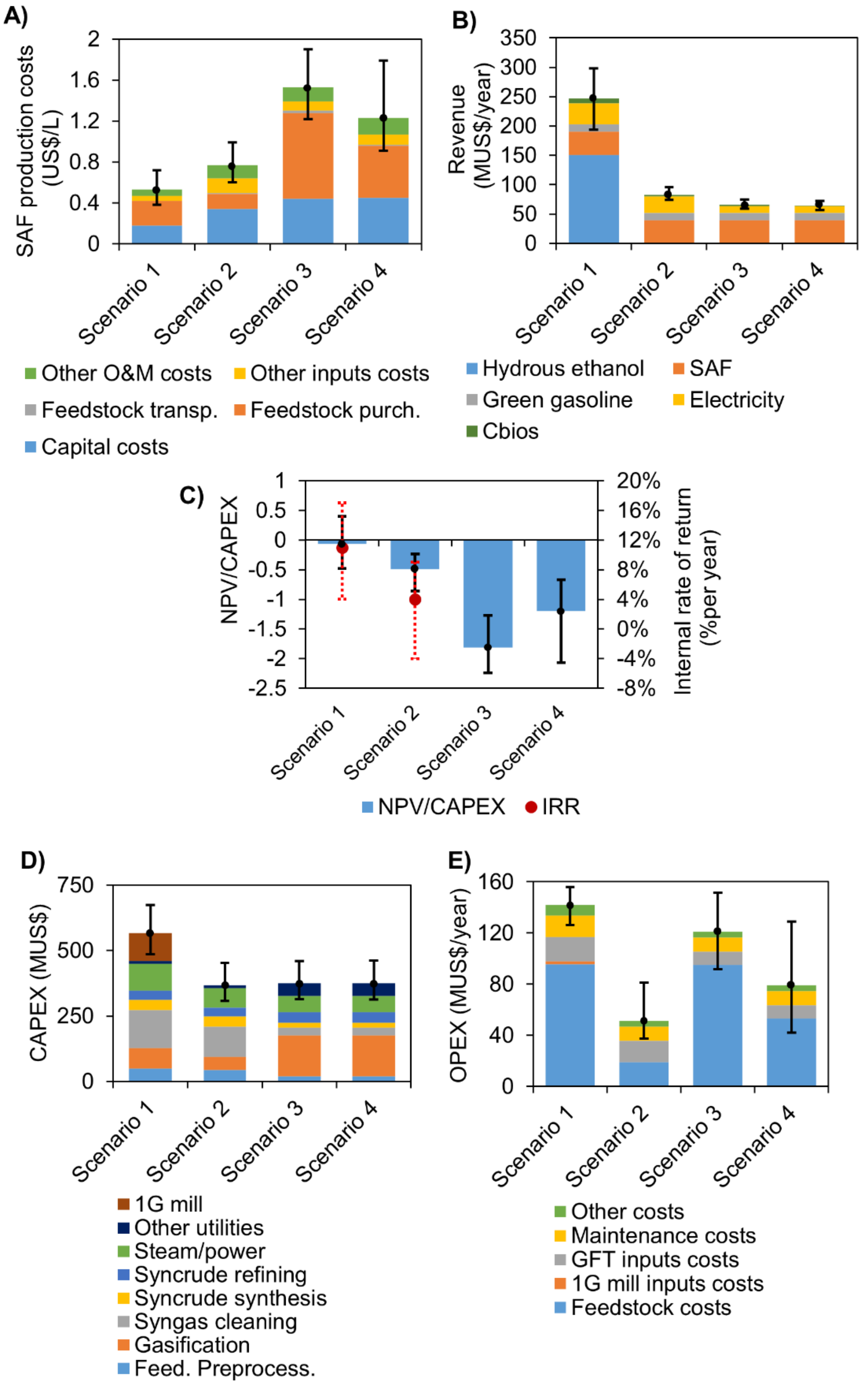


Figure V-5 – Economic results for the production of SAF: (a) SAF production costs breakdown (US$/L); (b) NPV/CAPEX and IRR investment; (c) annual revenue breakdown (MUS$/year); (d) total investment breakdown (MUS$); (e) annual operational costs breakdown (MUS$/year).

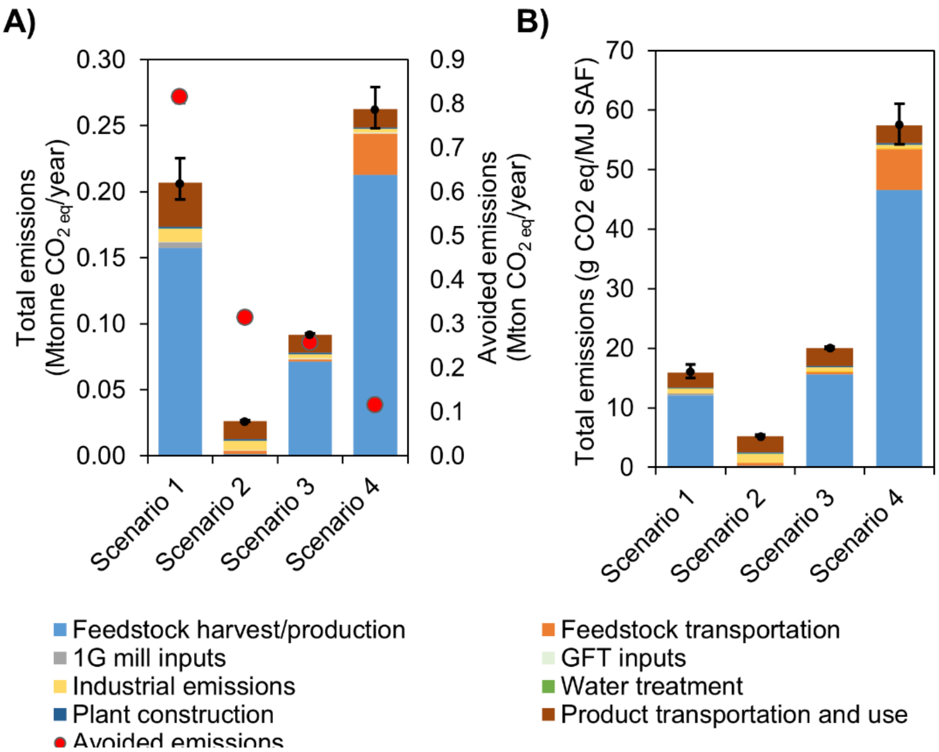


Figure V-6 – Main environmental results for SAF production: total emissions breakdown in (a) Mtonnes $CO_{2\ eq}$/year and (b) Mtonnes $CO_{2\ eq}$/MJ of SAF

Overall, the average range for the SAF production costs is between 0.54-1.54 US$/kg, or 11.33 – 32.31 US$/GJ (Figure V-5.a). These values are within the range observed in the literature. Usual values for FT fuels are around 1.1 – 3.19 US$/kg [61,62] or 18.6 – 33 US$/GJ [8,63,64]. However, it is important to notice that the selling price for FT fuels, in general, can vary widely based on feedstock and plant capacity [5].

Scenario 1 corresponds to the highest investment costs and annual operational expenses among all scenarios (Figure V-5.d and Figure V-5.e, respectively), as a result of the operation of the 1G mill alongside the thermochemical unit. However, this is by far the best scenario in terms of economic performance (Figure V-5.c) and avoided emissions (Figure V-6.a). The commercialization of ethanol significantly raises revenues (Figure V-5.b), while also increasing the total avoided emissions from the substitution of fossil fuel on the market. The added revenue from ethanol and the additional CBios is enough to ensure that this is the only scenario able to achieve a range of economic feasibility (IRR = 12 %/year, or NPV = 0, as shown in Figure V-5.c).

The ethanol production also indirectly influences the OPEX of Scenario 4, as shown by its lower operational costs compared to Scenario 3 in Figure V-4.e. As Scenarios 3 and 4 share the same GFT process configuration, the only difference between both cases is the integration of the FP process with the 1G mill unit. This integration leads to lower bio-oil production costs and a decrease in the selling price thanks to the additional revenue from ethanol, similar to the trend in Figure V-4.a, Section 3.1.

Investment costs are similar for Scenarios 2, 3, and 4 as observed in Figure V-5.d. Scenarios with bio-oil (Scenarios 3 and 4) have higher costs associated with the gasification step, a result of using higher complexity and pressurized reactor. However, as pointed out by Zheng et al. [65], bio-oil gasification produces less tar, and the water present in the reactor can react with tar via steam reforming reactions. Not only that, but the syngas obtained from bio-oil is almost free of particulate matter and ashes. The production of cleaner gas reflects lower costs with cleaning since fewer treatment steps are necessary. As a consequence, the total investment of the bio-oil gasification cases (Scenarios 3 and 4) is practically equal to that of the LCM gasification case (Scenario 2). The main cause for the difference in economic performance between these three cases is the higher feedstock costs in Scenarios 3 and 4 (Figure V-5.a).

Figure V-5.c shows that Scenarios 3 and 4 have slightly lower revenues compared to Scenario 1, which is due to lower electricity production in the former. The absence of equipment such as catalyst regenerators and char combustors for the bio-oil GFT configuration results in fewer hot streams available for the process. These streams are useful for heat transfer and steam/electricity production. As for the operational costs, Figure V-5.e highlights that feedstock highly influences the total cost. Brazilian LCM is relatively cheap (bagasse and straw), and its densification into bio-oil adds costs to the feedstock.

The feedstock also presents a large influence on the emissions of each scenario. From Figure V-2.c and Figure V-2.d (Section 3.1), it can be noticed that GHG emissions from sugarcane stalk harvesting are considerably larger than for straw harvesting. Figure V-6.a clearly shows that the total emissions of Scenario 1 are highly dependent on the feedstock acquisition since the LCA attributes the emissions from the feedstock to the final product. The same is also observed for Scenario 4 since, for this configuration, the FP unit is integrated into a 1G mill. In this manner, the emissions from sugarcane harvesting are incorporated into the thermochemical processes where integration takes place, namely the biomass gasification in Scenario 1 and bio-oil production in Scenario 4.

To illustrate the importance of the RenovaBio policy, Figure V-7 presents the influence of the CBios price on the economic feasibility of each scenario, measured as a function of the NPV normalized by the total investment (NPV/CAPEX). Logically, the higher the carbon price promoted by this policy, the better the results for all scenarios. This was observed by Bressanin et al. [66] in the study of different configurations for electricity production. For scenarios with production of biofuels (ethanol on 1G mill, and liquid fuels from the GFT route), the higher the value paid for avoided emissions, the higher the revenues and IRR. For the present study, the increase in the CBios price is enough to make Scenario 2 viable. Scenarios 3 and 4 are still under the minimum acceptable return, however, even for carbon prices above 100 US$/tonne. Scenario 4 is less sensitive to the increase in the CBios price since this is the scenario with the least favorable environmental performance (i.e., with the highest biofuel GHG intensities, as shown in Figure V-6). Scenario 1 presents the best results from the increase in the CBios price, due to the substitution of fossil gasoline for ethanol produced in the 1G mill. As a result, even carbon prices of around 20 US$/tonne are enough to move this scenario into the zone of positive NPVs, while higher CBios make this configuration more economically attractive.

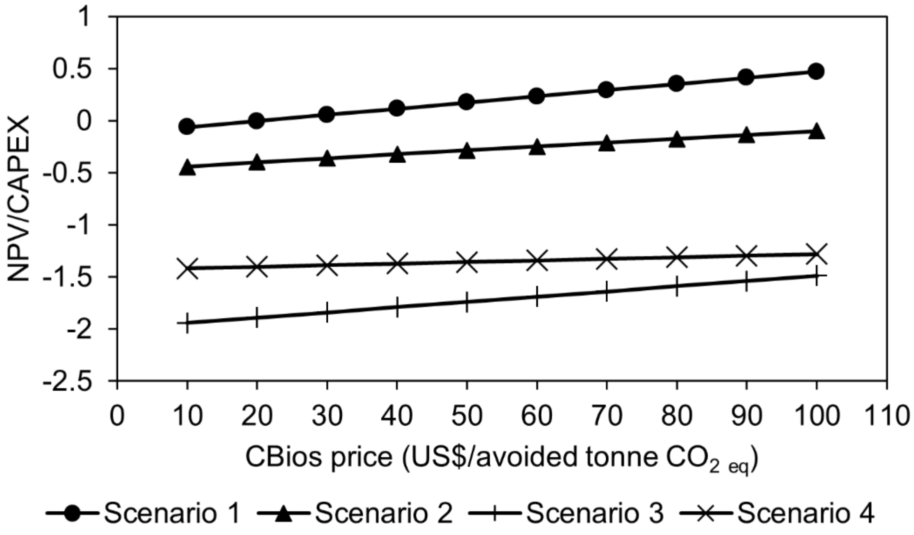


Figure V-7 – Influence of CBios price on the economic performance (NPV/CAPEX) of each scenario.

3.3. Decentralization analysis

The results obtained up to this point show that bio-oil is a more expensive feedstock than LCM biomass, especially by comparing Figure V-2.a and Figure V-4.a, and by the results in Figure V-5.e. The benefit of densification is mainly related to the lower transportation costs; however, the share of transport costs is relatively low both in the total production costs (Figure V-5.a) and total emissions (Figure V-6.a). This is due to the relatively shorter distances considered in the base scenario (below 100 km), thus making decentralization not an attractive strategy from a techno-economic standpoint.

Since bio-oil presents higher production costs, the decentralization option would only be more competitive if much longer distances were required. In this case, the consequent decrease in transportation costs would offset the relatively higher feedstock costs. To better evaluate in which conditions decentralization would become more competitive, longer transport distances were tested in a sensitivity analysis. Figure V-8.a presents the total costs with feedstock and emissions for Scenarios 2, 3, and 4. For a transport distance of 0 km, there is only the influence of the feedstock costs since no transport is required. Scenario 3 has the highest costs, followed by Scenario 4 at 0 km, which demonstrates that FP bio-oil incurs higher feedstock costs for SAF production when compared to raw sugarcane biomass.

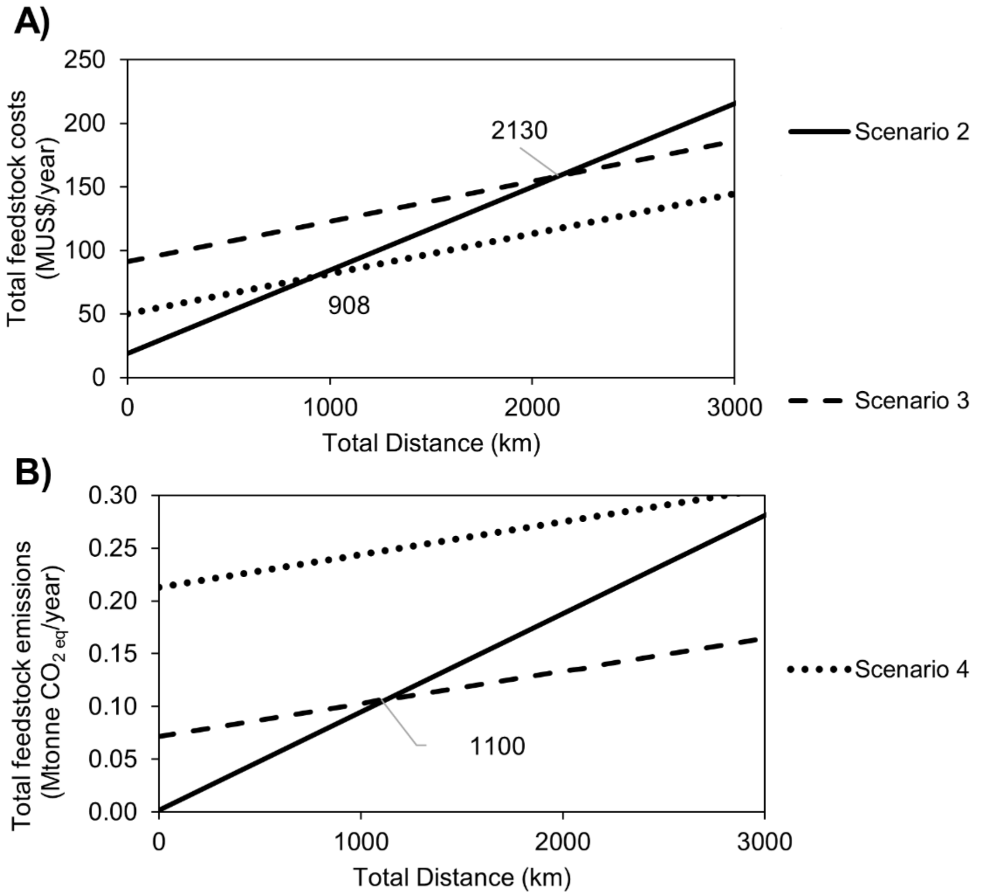


Figure V-8 – Influence of transportation distance on the (a) total feedstock costs and (b) total emissions with feedstock acquisition for Scenarios 2, 3, and 4.

As depicted in Figure V-8.b, for the GHG emissions, the acquisition of LCM alone (Scenario 2) presents almost no emissions, thanks to the zero-emission attributed to bagasse, and the lower emissions associated with straw (the biggest share of the impacts are allocated to sugarcane stalks, as seen in Figure V-2.c and Figure V-2.d). FP also increases the emissions for the feedstock, in a similar manner as the increased cost.

In Figure V-8, Scenario 2 shows higher variations both in feedstock costs and emissions as a function of the total distance, i.e., the slopes of the curves in Scenario 2 are larger than in other scenarios. The different behavior of the curves is associated with the higher costs and emissions from the solid LCM transportation than for the bio-oil. As a consequence, the feedstock cost of Scenario 2 becomes higher than those of Scenarios 3 and 4, for distances above 1,000 and 2,000 km, respectively (Figure V-8.a).

Similar behavior is observed for the total emissions with feedstock acquisition (Figure V-8.b) since, for distances above 1,000 km, the production and transportation of LCM exceed the emissions from the production and transportation of bio-oil in Scenario 3. Although Scenario 4 presents the worst environmental results with the highest GHG emissions up to transportation distance of 3,000 km (Figure V-5.c), the centralized LCM gasification would represent a higher impact than the decentralized scenario for distances above 3,000 km.

Thanks to lower emissions for longer distances, the decentralized cases (Scenarios 3 and 4) could benefit more from the CBios market. Lower emissions during transportation would result in higher avoided emissions and, consequently, higher revenues from carbon credits. If the CBios price rose above the average of 10-20 US$/tonne, the lower emissions of the decentralized scenarios would make them even more attractive than the centralized GFT if long distances of biomass transportation were involved.

Considering the concept of a distance above which the decentralization becomes more attractive both economically and environmentally in terms of feedstock acquisition, Figure V-9 expands the analysis of Figure V-8 by considering different industrial processing capacities and changes in CBios price.

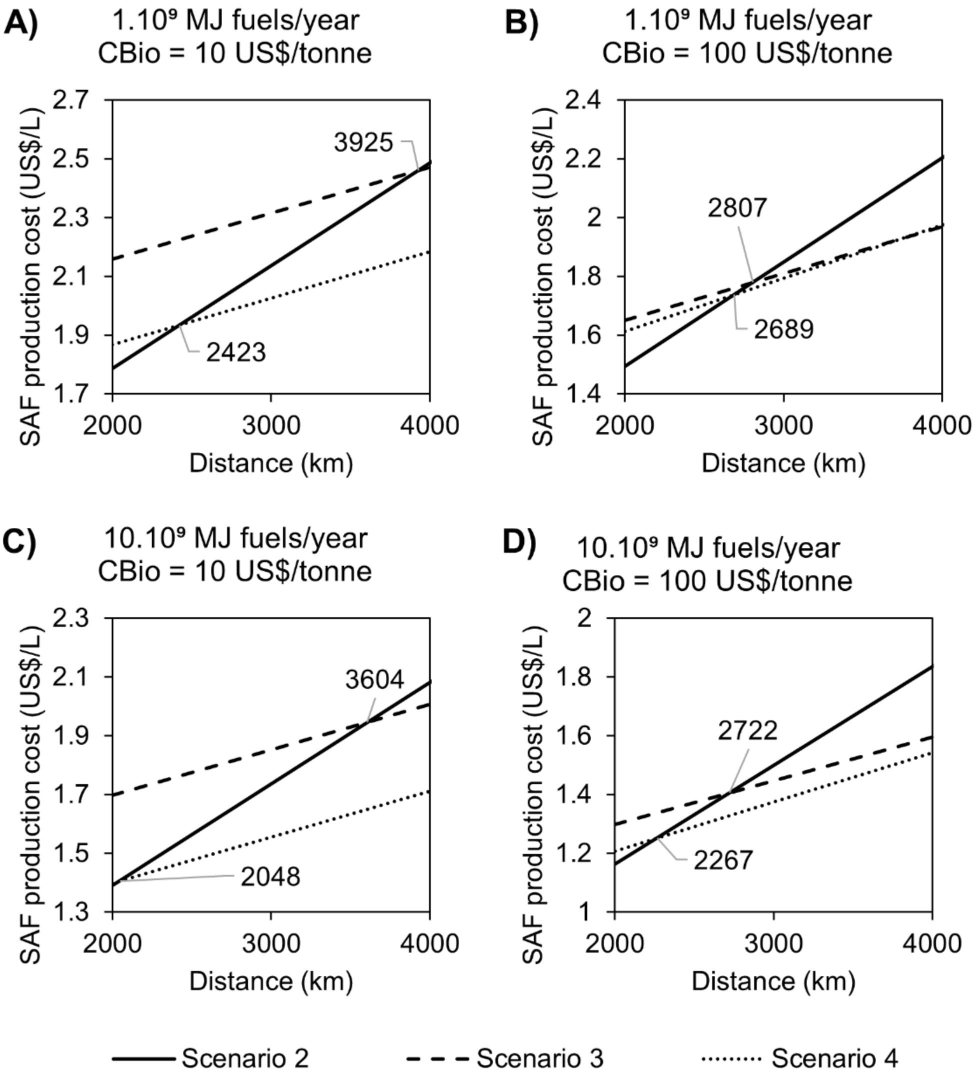


Figure V-9 – Influence of transportation distance, capacity, and CBios price on the total production cost of SAF in Scenarios 2, 3, and 4.

The first case (Figure V-9.a) represents the lowest scale – 1.10^9 MJ of liquid fuels/year – and the average CBios price – 10 US$/tonne. For these considerations, Scenario 4 has lower SAF production costs than Scenario 2 for distances above 2,423 km. For Scenario 3, this distance is equal to 3,925 km. These results indicate which distance between the biomass production site and the final conversion to SAF would justify the implementation of FP densification units rather than relying on a single centralized LCM GFT plant.

As mentioned previously in Figure V-8.b, bio-oil transportation also represents lower emissions, and the use of CBios may improve the competitiveness of the decentralized scenarios. Figure V-9.b shows the influence of increasing the value for CBios to 100 US$/tonne. This increased revenue from carbon credits benefits all the scenarios; however, scenarios with higher avoided emissions benefit more from this change. The SAF production costs decrease about 20% in Scenarios 2 and 3, but only around 10% in Scenario 4 since the latter has less avoided emissions (Figure V-5.c). Thus, Scenario 4 only presents lower production costs than Scenario 2 for distances above 2,689 km (longer distances than those observed in Figure V-9.a), whereas this distance shortens to above 2,807 km (compared to over 3,500 km in Figure V-9.a) in Scenario 3.

Figure V-9.c illustrates the influence of increasing the capacity of the plant to 10.10^9 MJ of liquid fuels/year. By comparing Figure V-9.a and Figure V-9.c, the increase in capacity lowers the distance in which the scenarios with decentralization (Scenarios 3 and 4) present lower SAF production costs than the centralized scenario (Scenario 2). More biomass is necessary to produce more biofuels, and thus, the increased demand for LCM reflects higher transportation costs for Scenario 2. Similar to the influence of the CBios price, where higher carbon prices benefit more scenarios with higher avoided emissions, the increase in capacity benefits more the cases with lower transportation costs.

The change from Figure V-9.c to Figure V-9.d indicates the same pattern observed when shifting from Figure V-9.a to Figure V-9.b, where the benefits from the CBios price are more relevant to Scenarios 2 and 3 than in Scenario 4.

Nonetheless, the results demonstrate that the decentralization strategy is unlikely to be economically attractive for the Brazilian sugarcane industry. To illustrate this point, with an area of approximately 250,000 km² (or a radius of less than 300 km), the São Paulo State was responsible for producing more than 350 Mtonnes of sugarcane for the harvesting of 2020/2021 [67]. Considering the overall yield of Scenario 1, this amount of biomass could produce over 300.10^9 MJ of liquid fuels from the GFT route. This is also for a mean transportation distance considerably shorter than those pointed out in Figure V-9. This panorama relates to the dense distribution of sugarcane in Brazil, where the Southeast region of the country is responsible for over half of the national production [48]. This region is also associated with the largest ethanol consumption in the country, and the biomass production sites are located near the main fuel markets. Therefore, this context discourages the decentralization of the production chain. Further studies should assess the decentralization of densified feedstocks for different regions of the country where a combination of lower availability of biomass and increased local biofuel consumption would justify longer transport distances.

4 - Conclusions

The use of the thermochemical route of biomass GFT to produce renewable and clean jet fuel presented promising results to help achieve the directives of net zero emissions by 2050. However, even with around 80 g $CO_{2\ eq}$ avoided per MJ of SAF produced, a standalone plant processing lignocellulosic biomasses still is not economically viable, achieving IRR values below 10% per year. With lower return on investment (negative net present values), such a configuration is not yet attractive for investors that still prioritize the economic perspective rather than its environmental benefits.

The reliance on governmental policies and subsidies can convert environmental performance into higher economic returns. However, a standalone GFT plant would depend on a carbon price as high as 140 US$/tonne $CO_{2\ eq}$ avoided to become competitive with the fossil option. The integration of the GFT route into the first-generation ethanol distilleries for the Brazilian scenario leads to better economic results without relying too much on high carbon prices. This configuration brings down the production costs of SAF to a competitive level (as low as 0.39 US$/L) with subsidies at the current market level.

On the other hand, the decentralization of the production chain did not achieve promising results. With investment costs of the same magnitude as the standalone GFT plant processing LCM, the bio-oil gasification unit ends up processing a feedstock twice as expensive as straw and bagasse. Even lower transportation costs were not enough to offset the high cost of purchasing bio-oil. The decentralization with smaller FP units would only reach lower production costs than the centralized GFT plant for distances way over 1,000 km.

The present work considered the particular scenario of the Brazilian sugarcane market, and further studies are required to evaluate which scenarios would benefit from decentralization – such as by focusing on regions with sparser biomass availability, or even by considering the use of other densification options.

The results here presented point out that including biomass densification in the production chain of SAF leads to an increase in feedstock costs and total emissions. Therefore, the best way to help develop the evaluated scenarios lies in both the integration of BtL plants into more mature biofuel production technologies (such as 1G ethanol production, which is an already established production chain) and by decreasing the GHG intensity of the biofuels produced to maximize the benefits from incentive policies such as RenovaBio. This pathway relies on the effort of both policymakers and investors alike if the demands for renewable energy and the reduction of emissions are to be achieved in time.

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Chapter VI - Discussion

1 - Additional results

Overall, the previous chapters followed a sequence, each building up on and expanding the discussion on the previous one. While Chapter III presented a review of the main bottlenecks for the GFT route, Chapter IV presented further details and expanded the analysis of the base case proposed on Chapter III from a techno-economic perspective. Besides including the life cycle assessment perspective, Chapter IV compares standalone and integrated configurations of the GFT plant. The conclusions clearly show the benefit of integrating the thermochemical route into the biochemical route of ethanol production.

Chapter V goes beyond this analysis and presents one of the key elements of the project, encompassing the topics of route integration and decentralization of the production chain for Sustainable Aviation Fuel (SAF) production. With this contribution, Chapter V presents a more detailed discussion of scenarios by complementing much of the discussion in Chapters III and IV.

However, some points addressed in these papers still have room for an expanded discussion, as some analysis could not fit in our previous research papers. Therefore, this chapter aims to elaborate on some of this analysis and help to improve the understanding of the work done. For this purpose, the present chapter presents further results for the fast pyrolysis process and the sustainable aviation fuel (SAF) production route.

For the present discussion, the nomenclature for the different scenario from Chapter V will be maintained: Scenario 1 is the integrated GFT into 1G mills; Scenario 2 is the standalone LCM GFT plant; Scenario 3 the standalone GFT plant processing bio-oil from a standalone FP plant; and Scenario 4 the standalone GFT plant processing bio-oil from integrated FP units (Figure V-1).

1.1.Fast pyrolysis densification units

Important aspects that are briefly discussed in Sections 2.2.4 and 3.1 from Chapter V are the considerations made to estimate the production costs and selling price of bio-oil. Since there is no well-developed market for this intermediate energy carrier, we consider that the minimum selling price of bio-oil will be defined by a situation in which the Standalone Plant's Internal Rate of Return (IRR) must reach at least the minimum acceptable rate of return (MARR) for the sugarcane industry (12% per year). However, for the integrated FP/1G mill plant, we assume that the minimum selling price of bio-oil is defined by a condition in which its IRR aim for at least the IRR from a standalone 1G mill. This approach embeds the idea that one investor would only integrate its current 1G mill to a new FP facility if the result of such integration provided at least the same IRR of his previous investment (1G mill). By establishing the integrated plant with the same return of a 1G mill, the investment into the FP unit is more competitive than if the return was set to 12% per year. This approach leads to more rigorous criteria for the integrated scenario, but the objective of this analysis is to propose an attractive investment option in comparison to the "base investment" (a 1G mill). Besides that, if we would adopt a requirement of 12% of return per year, there are scenarios in which the 1G mill alone would achieve IRR>16% per year. This performance of the mill would allow the bio-oil to be sold at "negative" prices to achieve returns of 12% per year. Thus, we also stablished the scenario of equivalence to the 1G mill in order to avoid this unrealistic behavior.

Figure VI-1 presents the difference between these two approaches for estimating the minimum selling price of bio-oil in the integrated scenario. It is clear that the consideration of matching the performance of an existing 1G mill is more demanding, since the plant is required to achieve a higher IRR (and therefore, higher NPV, as seen on Figure VI-1.a). By taking into account the results presented on Table VI-1, the commercialization of bio-oil has to compensate these higher costs since the total investment and operational costs of an integrated plant is higher than for a 1G mill. Thus, as depicted in Figure VI-1.b, both the production costs and selling price of the bio-oil are considerably higher by leveling the performance of a 1G mill than by stipulating a MARR of 12% per year.

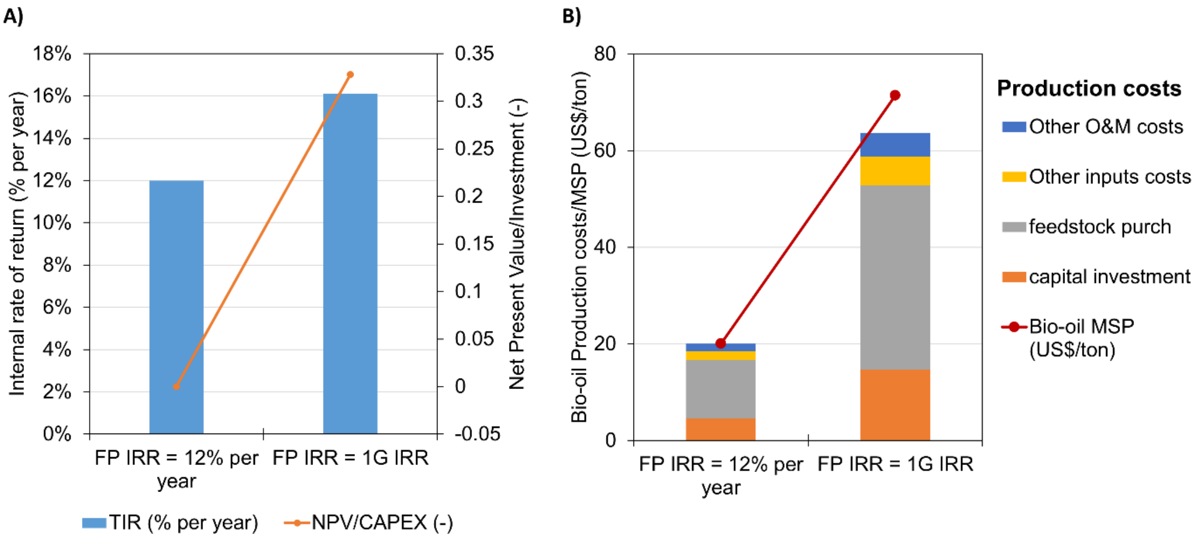

Figure VI-1 - Comparison for the options of bio-oil pricing for an integrated FP plant. (a: IRR and NPV/CAPEX of the FP plant; b: Bio-oil production costs and minimum selling price)

Table VI-1 - Comparison of the main economic results of 1G mill, and standalone and integrated Fast pyrolysis plant

	1G mill	**SA FP**	**INT FP/1G**	
CAPEX	237	198	298	MUS$
OPEX	108	44	122	MUS$/year
Production				
Hydrous ethanol	350	-	350	10^6 L/year
Bio-oil	-	0.42	0.42	Mtonne/year
Electricity	0.24	0.53	0.23	10^6 MWh/year
CBios	0.47	-	0.56	10^6 ton avoided CO_{2eq}/year/

Another impact of choosing between these criteria are perceived on the uncertainty of scenarios, as explained on Chapter V (section 2.7). Figure VI-2 presents the variation of the IRR of a standalone 1G mill considering the range for the parameters described in Table V-1 (Chapter V, section 2.7), while Figure VI-3 shows the resulting bio-oil production costs and minimum selling price for the pessimistic, base, and optimistic cases considering both FP plant IRR = 1G mill IRR and 12% per year (MARR). These optimistic and pessimistic scenarios are evaluated based on more extreme values as represented in Table V-1, in a similar fashion to Table III-8.

Figure VI-2 depicts the variation of the IRR from a 1G mill, whose results can range from negative values to approximately 25% per year. This has a peculiar influence on the behavior of the integrated FP unit if the bio-oil production had to achieve an equivalent economic performance. For the optimistic case (Figure VI-3.a), bio-oil has to be sold at a price 23% higher than the base scenario in order to keep up with the high return for the 1G mill caused by more extreme variations in the maximum ethanol price (up to +33%, as depicted in Table V-1). This occurs even though bio-oil production costs are lower when compared to the base case. For the pessimistic case, production costs are 13% higher than the optimistic case, but remains lower than from the base case, with a decrease of 48% in the bio-oil minimum selling price. The need of matching the economic returns from the previous 1G plant is responsible for this behavior. Since for the pessimistic scenario for the standalone 1G mill reach negative IRR (Figure VI-2), the bio-oil can be sold at lower prices to match this poor performance. This behavior shows that the bio-oil commercialization has to be increased in order to reach the performance of an optimal 1G mill, while the restriction is more lenient for the pessimistic considerations.

Such an occurrence is not observable when the MARR is set to 12% per year (Figure VI-3.b). For this stipulation, the pessimistic scenario corresponds to production costs and selling price over 9 times higher than for the base scenario. For this pessimistic scenario, much of the weight to aim for 12% per year depends on the commercialization of bio-oil since the IRR of a 1G mill achieves negative values (Figure VI-2). Thus, both the production costs and minimum selling price of this intermediate see a sharp rise on their values. Alternatively, since the 1G mill’s IRR is high enough (above 20% per year) for the optimistic case, the bio-oil commercialization is less relevant to the revenue. Thus, the production costs and minimum selling price of the bio-oil for the optimistic scenario achieve negative values for a fixed MARR of 12% per year.

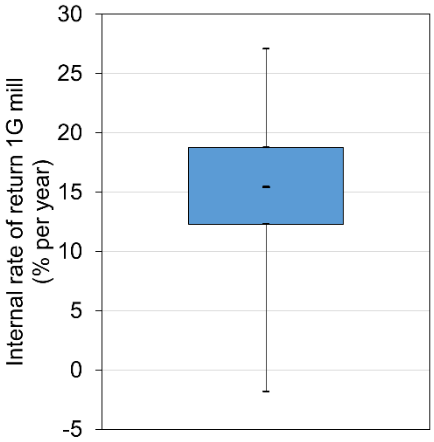

Figure VI-2 –Variation of internal rate of return of a 1G mill from the uncertainty analysis

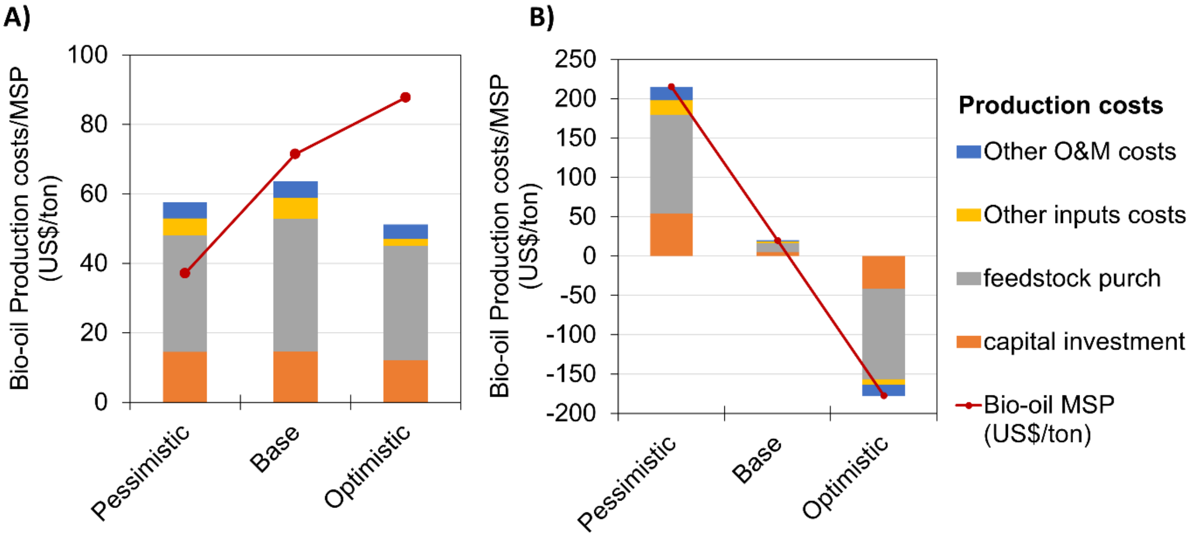

Figure VI-3 –Range of bio-oil production costs and minimum selling prices for the pessimistic, base and optimistic scenarios from the uncertainty analysis.(a: matching the IRR of the integrated plant to the 1G mill; b: fixing the MARR of the plant to 12% per year)

From these observations, the analysis on Chapter V considered that the commercialization of bio-oil from an integrated plant should be competitive with a standard 1G mill, and always maintain a minimum return of investment which is attractive enough to the investors. These criteria stablish that the integrated plant should match the 1G mill's IRR in the cases wherein it is above 12% per year; otherwise – for conditions in which the mill would perform below the minimum return – the INT FP unit IRR is fixed to 12% per year. Figure VI-4 presents the results from these considerations based on the bio-oil production costs and minimum selling prices in the uncertainty analysis. We verify that the increased investment and operational costs of the pessimistic scenario leads to production costs and minimum selling prices three times as high as those for the base considerations. This is a consequence of bio-oil being responsible to reach the 12% per year MARR, since the performance of the standalone 1G mill would achieve negative IRR values (Figure VI-2). For an optimistic scenario, the production costs are 76% and 20% lower than the pessimistic and base scenarios, respectively. However, the bio-oil minimum selling price is 23% higher than for the base considerations, since the bio-oil commercialization has to match the high IRR of the 1G mill as observed on Figure VI-2.

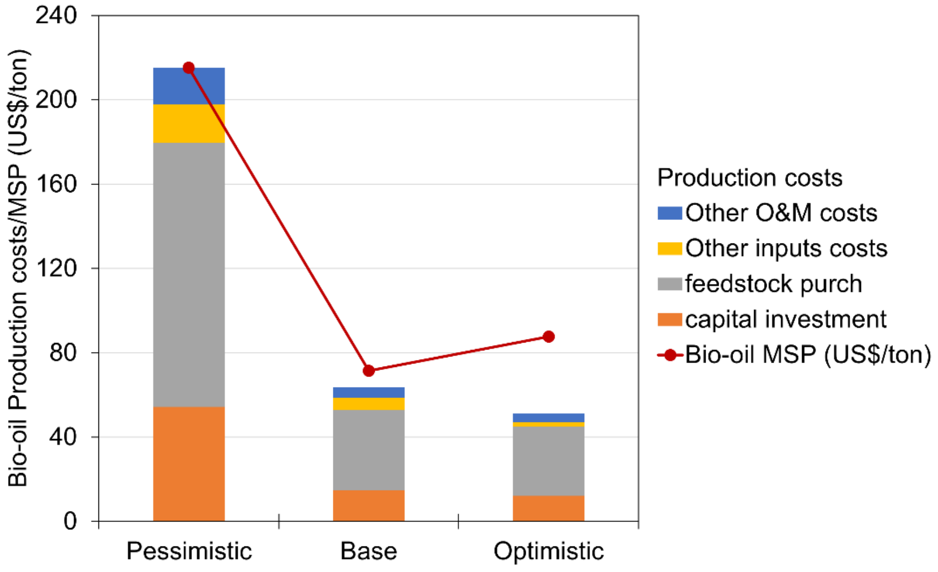

Figure VI-4 – Range of bio-oil production costs and minimum selling prices for the pessimistic, base and optimistic scenarios from the uncertainty analysis – adopted criteria

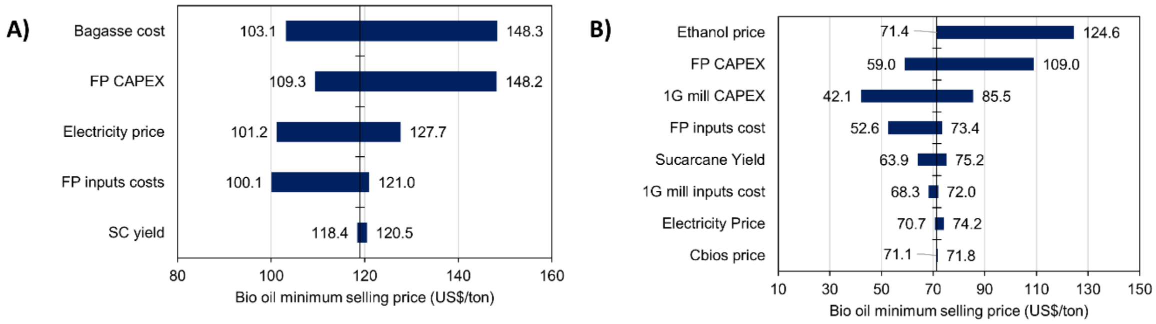

Figure VI-5 – Tornado diagram for both FP scenarios (a: standalone plant; b: integrated plant)

From Figure VI-5.a, bagasse cost is the most influential parameter for bio-oil minimum selling price on the SA configuration both due to the importance of biomass price, and the considered range of variation for bagasse cost (4-21 US$/tonne, Table V-1). For the same configuration, however, the sugarcane yield is the least influential parameter, even though this factor is related to the sugarcane straw price. However, this influence is indirect, and the straw price is less pronounced than the bagasse. For the INT configuration (Figure VI-5.b) the influence of yield is more pronounced as a consequence of the higher cost of sugarcane stalks (Figure V-2.b), which can be over 70% more expensive than straw and bagasse in terms of energy.

As expected, ethanol price only influences the integrated configuration (Figure VI-5.b) and its variation leads to the largest changes on bio-oil MSP. However, this parameter only leads to an increase on the bio-oil minimum selling prices since this product has to fill the revenue gap left by the absence of higher ethanol prices. The CBios price has a similar effect, but a much lower scale of influence on the results (around 1% of difference). This parameter could become more relevant if higher prices of carbon credits were adopted, since only a small percentage of the revenue of the plant is attributed to CBios (under 6%).

For both scenarios, the fixed investment on the Fast Pyrolysis plant (FP CAPEX) is one of the most important parameters. This is expected since CAPEX is alone responsible for around 30% of the production costs of bio-oil Figure V-4.a. Chapter III already presents a discussion of a similar behavior from the GFT plant (Figure III-4) as a result from the higher investment on these thermochemical routes. The 1G mill CAPEX variation lead to variations of up to 60% on the bio-oil production costs. This is different of the analysis for the GFT (Figure III-4), where the mill investment was not that influential. For comparison, the 1G mill fixed investment corresponds to around 40% of the total CAPEX of the total CAPEX of the INT FP plant (Figure V-4.c), while for the INT GFT plant this value is less than 20%.

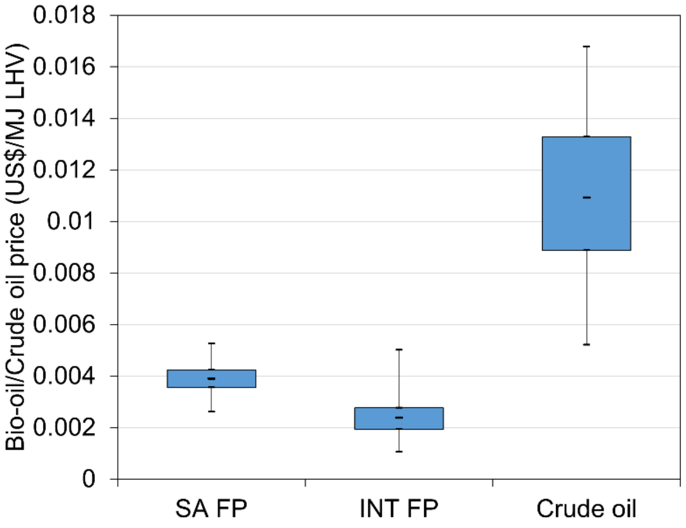

Figure VI-6 –Comparison, of bio-oil minimum selling price and crude oil historic price

Figure VI-6 presents a comparison between the bio-oil minimum selling prices for both SA and INT scenarios and compares these results to the historic variation of crude oil prices on an energy basis (lower heating value, LHV). This study estimates crude oil prices according to data from the IPEA (2022) for the past 10 years. These results point out to a relatively low price of bio-oil, especially when taking into account the discussion on Chapter V (Section 3.1) whose production costs were below those observed in the literature for bio-oil (VASALOS et al., 2016; LI et al., 2017; SHAHBEIG and NOSRATI, 2020).

Regardless of the relatively lower MSPs obtained in this study, this still is not a clear indication that the bio-oil produced from the proposed technological configurations is competitive with crude oil. The FP process configuration in the present study accounts only for the separation of co-products (gases, condensable and solids) and a light stabilization process with methanol to prevent aging of bio-oil. Compared to similar studies, the present bio-oil is not upgraded, and its combustion properties are far from being equivalent to crude oil.

The present study only takes into account the use of bio-oil as an intermediate to produce a narrow range of products (mainly SAF and green gasoline). On the other hand, crude oil processing presents a larger array of products. Instead of comparing the production costs in terms of mass or energy, a better comparison between bio-oil and crude oil should consider the final use of these energy carriers. By taking into account the products obtained from the processing of these materials, it is possible to evaluate the possible advantages of the renewable option. For example, one possibility is processing bio-oil similarly to crude-oil. Some studies point out at the possibility of co-processing bio-oil into existing petroleum refineries' fluid catalytic cracking (FCC) units at a proportion of up to 20% of raw bio-oil (BHATT et al., 2020). By pricing the bio-oil based on the potential liquid fuel production it would lead to a better comparison with crude-oil and among other intermediaries. However, further studies would be required to assess the economic impacts of such type of bio-oil upgrading.

1.2.Sustainable aviation fuel production

Figure VI-7 expands the results discussed on Chapter V by considering the sensitivity analysis similar to Chapter III (Figure III-4 and Figure III-5) for the range of variation from Table V-1. From these results, the GFT CAPEX is particularly important for all scenarios and for both the economic feasibility (NPV/CAPEX) and the SAF production costs. As stated previously, both on Chapter III and on the discussion for the FP (Section VI.1.2), the CAPEX of the thermochemical processes is elevated and increases the importance of this parameter for the project's economic performance.

Another important parameter is the cost with feedstock. For Scenario 1 (Figure VI-7.a and b) the sugarcane yield (SC) is reflected on the price of sugarcane, and it corresponds to a significant degree of influence on both NPV/CAPEX and SAF production costs. The variation on this parameter can lead to changes of up to 8% of the SAF production costs. This is thanks to the large share of expenses attributed to feedstock purchase (Figure III-2 and Figure V-5) on this scenario, where biomass production corresponds to 45% of total costs. Feedstock also presents large influence on Scenario 2 in the form of bagasse cost (up to 14% of influence on SAF production costs). However, SC yield is less influential due to the indirect correlation to straw price, corresponding to below 1% of influence on SAF production costs. The results for Scenarios 3 (Figure VI-7.e and f) and 4 (Figure VI-7.g and h) are largely influenced by the bio-oil price due to the large costs with this feedstock (Figure V-5.a). For example, the variation of bio-oil price can lead to changes of up to 30% and 50% on SAF production costs for scenarios 3 and 4, respectively.

In regards to the co-products besides aviation fuels, ethanol price is clearly important for Scenario 1 (Figure VI-7.a and b) due to responding for over 60% of the total revenue of the integrated plant (Table III-6 and Figure V-5.c). On the other hand, green gasoline commercialization is one of the less influential parameters for every scenario due to the lower production of this fuel (below 20% of the revenue for all scenarios). Electricity commercialization is responsible for 34% of revenue from scenario 2, and below 17% for all the other scenarios. Thus, it follows that electricity price is more important on Scenario 2 than for the other due the difference on production of surplus electricity.

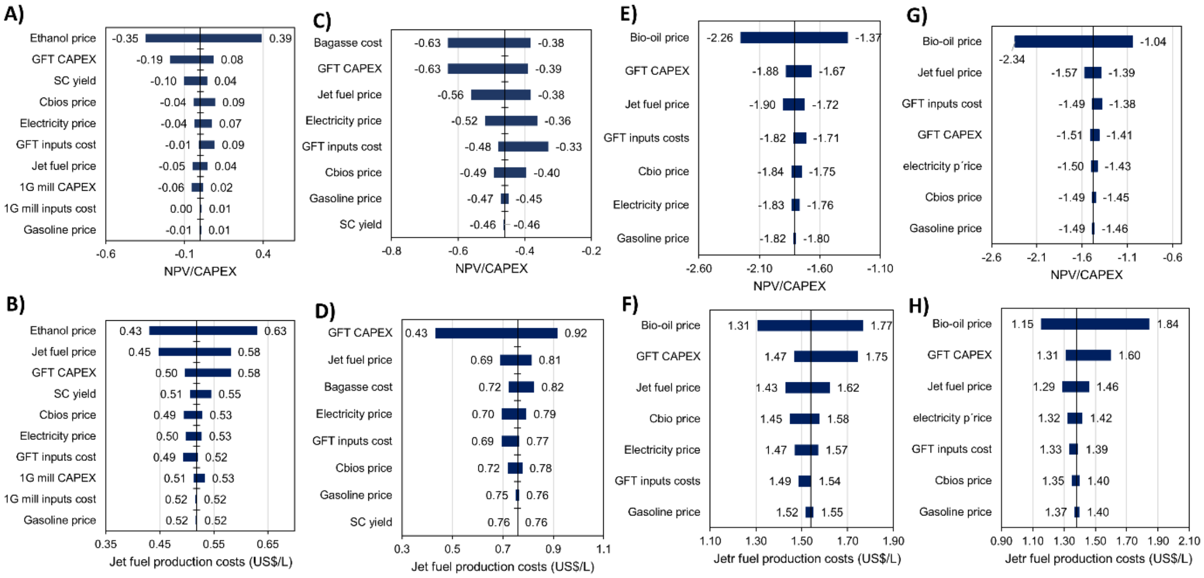

Figure VI-7 – Tornado diagram for the different scenarios for SAF production (Scenario 1 – a: NPV/CAPEX, b: SAF production costs; Scenario 2 – c: NPV/CAPEX, d: SAF production costs; Scenario 3 – e: NPV/CAPEX, f: SAF production costs; Scenario 4 – g: NPV/CAPEX, h: SAF production costs)

Figure VI-8 presents the economic results for all scenarios considering the variation in the main parameters. These results allow to better illustrate the performance of each scenario, and it is possible to observe that clearly Scenario 1 presents the best results. Even with higher investment costs (Figure VI-8.a) and operational costs on the top range of observed values

(Figure VI-8.b), the total revenue (Figure VI-8.c) more than compensates these costs with the results of NPV (Figure VI-8.e and e).

As previously discussed on Chapter V (Section 3.2) the scenarios with bio-oil production are hindered by high operational costs from the expenses with the feedstock. This is evident since these scenarios present similar investment costs to Scenario 2 (Figure VI-8.a) whereas presenting operational costs almost at the level of Scenario 1 (Figure VI-8.b). Not only that, but Scenarios 3 and 4 also represent a wider range of variation for operational costs due to range of bio-oil minimum selling prices (Section VI.1.1), which vary from 90-176 US$/ton and 26-160 US$/ton for the SA and INT configurations, respectively. This brings a higher degree of uncertainty for these scenarios, as can be seen on Figure VI-8.d and e for the values of NPV, which can present a range of variation above 70%. On the other hand, Scenario 2 presents the narrowest variation between the different scenarios since only the parameters directly related to the GFT influences it.

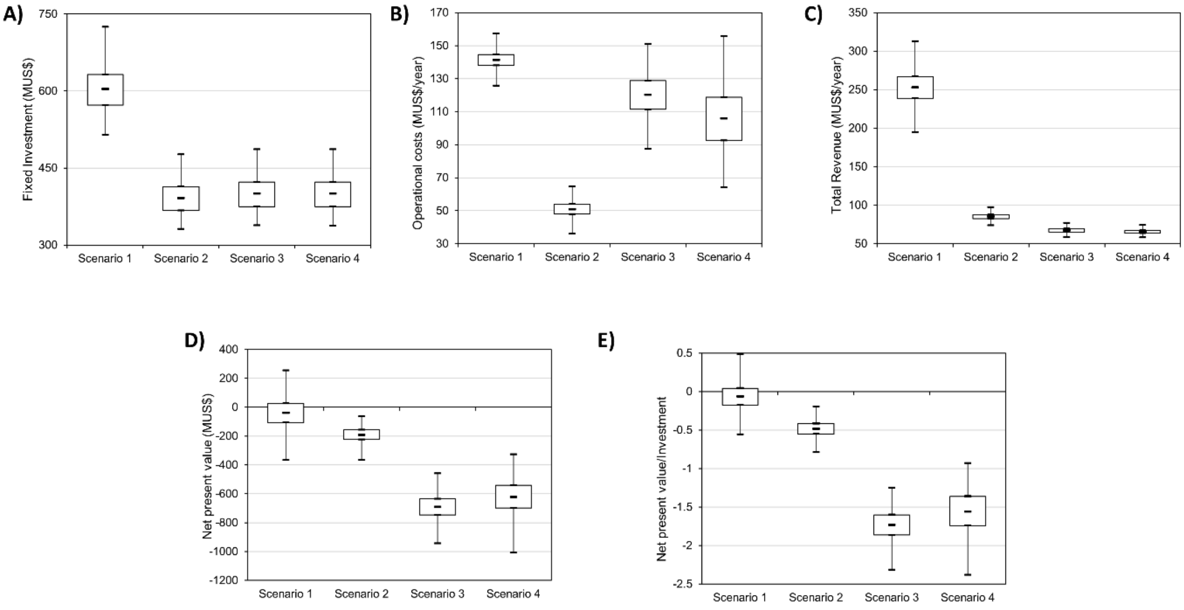

Figure VI-8 –Boxplot for the uncertainty analysis for the different SAF production scenarios (a: Fixed Investment; b: Annual Operational costs; c: Total annual revenue; d: Net present value; e: NPV/CAPEX)

Concerning the environmental performance of these scenarios, Figure VI-9 presents the results for total and avoided GHG emissions. From Figure VI-9.a, Scenarios 1 and 4 present the largest total emissions due to sugarcane production, i.e., harvesting stage to be more specific, which contributes with over 70% of overall emissions for scenario 1. The influence for scenario 4 is more indirect, since the sugarcane production emissions are allocated to the bio-oil produced on an INT FP plant.

When avoided emissions are considered, Scenario 1 is responsible for a large share of fossil fuel substitution due to ethanol production, which is responsible for around 70 g of CO_{2eq} avoided per MJ of ethanol produced. Scenario 4, however only counts with SAF and a small amount of green gasoline, thus presenting the worst environmental performance (Figure VI-9.b), with total avoided emissions 86 % lower than scenario 1.

If we only consider the avoided emissions by SAF substitution (Figure VI-9.d), Scenario 2 presents the lowest total emissions among the different scenarios, approximately 80 gCO2eq MJ-1. Even though Scenario 1 presents the highest total GHG avoided, much of this performance is attributed to ethanol, so only 70 g CO_{2eq} is avoided per MJ of SAF produced.

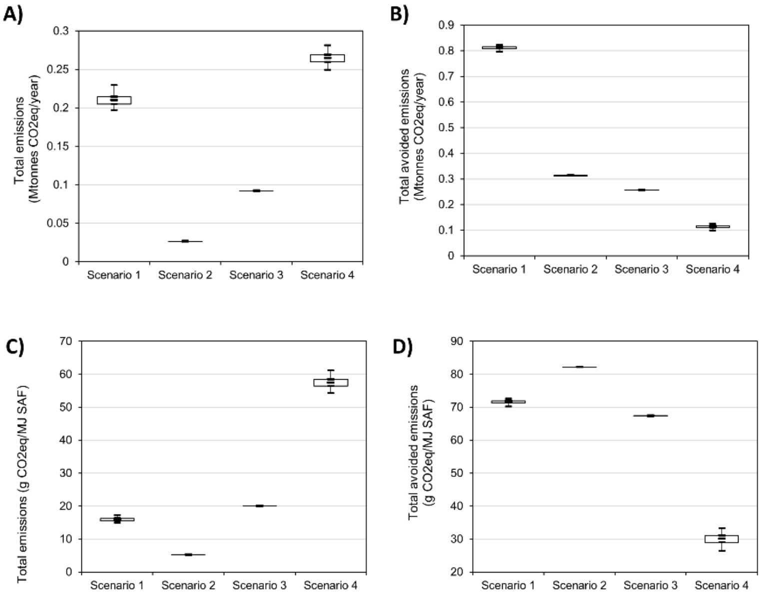

Figure VI-9 - Boxplot for the uncertainty analysis for the different SAF production scenarios (a: total annual emissions; b: total annual avoided emissions; c: total emissions/MJ of SAF; total avoided emissions/MJ of SAF)

2 - SAF production in the context of GHG emission mitigation

The main purpose of this study is to evaluate a technological scenarios capable of supplying a clean alternative for aviation fuel in order to achieve the different decarbonization targets from international agreements aiming at climate change mitigation in the aviation sector. In the national context, Brazil is determined by its NDC from the Paris agreement to reduce GHG emissions in 2025 by 37% compared with 2005, and by 50% in 2030 compared to the same basis (FEDERATIVE REPUBLIC OF BRAZIL, 2022).

For a narrower application focused on aviation, Brazil also takes part in the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA), a resolution from the International Civil Aviation Organization (ICAO) composed by more than 190 countries aiming to limit emissions from the civil flight sector. The main objective of this mechanism is to limit the GHG emissions to a fixed level fixed to the year 2020 (SOARES and CENAMO, 2018). With this target in mind, it is expected the carbon neutral growth of the international flight sector from 2020 onwards. The implementation of the CORSIA is planned in three stages: the first is a demonstration stage with only a few voluntary countries from 2021-2023; the second stage, from 2024-2026, is expected to count with more voluntaries; finally, from 2027 to 2035 the mandatory period begins, with all required countries taking part into the effort. Brazil is only expected to take part on the mandatory phase after 2027 (SOARES and CENAMO, 2018).

In order to achieve these determinations, all companies (national and international) offering international flights from and to Brazil are obliged to comply with the targets and take measures to mitigate their emissions accordingly. Figure VI-10 presents a projection of the compensation for emissions from the international flight sector in Brazil, based on the determinations from CORSIA (SOARES and CENAMO, 2018).

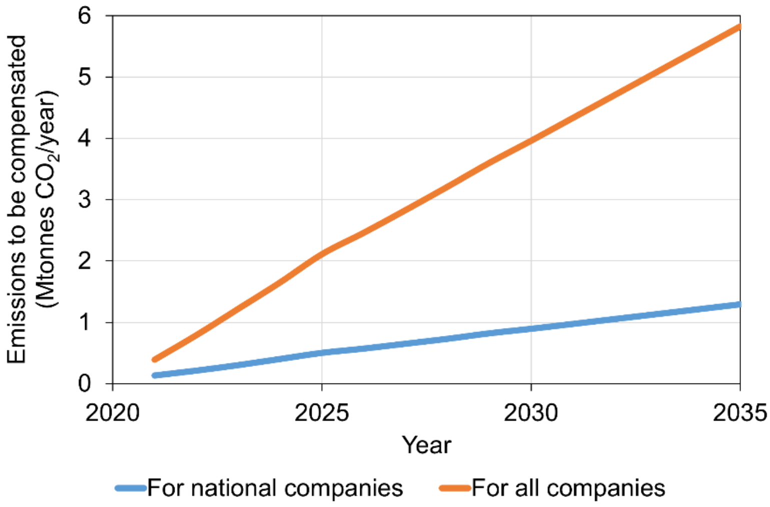

Figure VI-10 - Required compensation of emissions for national and international companies according to CORSIA determinations

Based on these projections for avoided emissions at national level and from our results presented in Figure VI-9, then we estimated the corresponding energy demand of SAF to be produced by each proposed scenario, and the required LCM to supply the production at Brazilian level (see Figure VI-11).

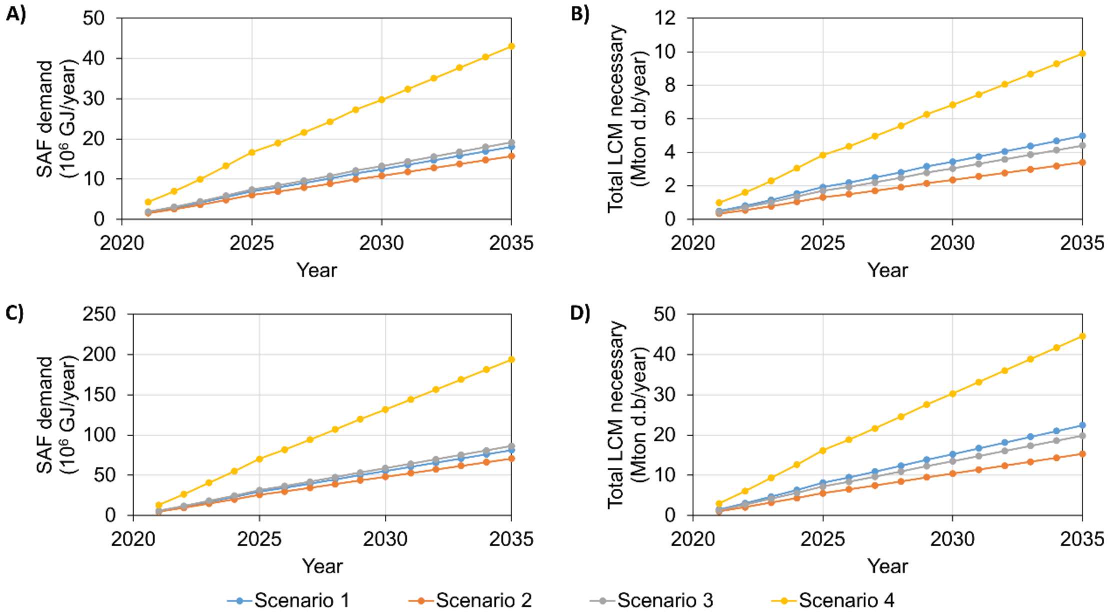

Figure VI-11 - Total SAF projected demand (a: for national companies; c: for all companies) and the required LCM production (b: for national companies; d: for all companies) to attend the CORSIA requirements

From these results, Scenario 2 presents the lowest amount of energy output required to meet the necessary GHG compensation at national level (approximately 16.10^6 GJ yr-1), due to the highest results for avoided emissions per unit of energy (as seen on Figure VI-9.d). Since Scenario 4 presents the highest GHG intensity among all scenarios, a higher use of LCM would be necessary as well as a larger production of SAF, with a production of over 40.10^6 GJ.yr^{-1} requiring around 10 Mtonnes of dry LCM per year. Thus, a larger substitution of jet fuel for SAF on the market would be necessary for scenario 4. Scenarios 1 and 3, however, present results similar to each other, with demand around 30% higher than for Scenario 2.

Considering the demand of SAF from national companies up to 2035 (presented in Figure VI-11.a), the number of required units for each scenario would be between 6 (Scenario 2) and 15 (Scenario 4), with each of these units as described on Chapter V (production capacities of 3.8 10^6 GJ liquid fuels per year). In other words, if the configuration proposed by Scenario 2 was chosen to supply the entire demand of SAF in the country, around 6 units as described on Chapter V would be necessary. If the less optimal environmental alternative (Scenario 4) was selected, however, 15 of these plants would be necessary. In terms of total biomass necessary,

Figure VI-11.b shows that around 3 to 10 M tonnes of dry LCM would be necessary each year, depending of the chosen configuration. Souza et al. (2021) performed a survey to evaluate the potential amount of available biomass in the Center-South region of Brazil. According to their results, for the 2018/2019 sugarcane season, around 50 M tonnes of straw (d.b.) were available to be recovered and used for bioenergy purposes in that region alone, even with some amount of the total produced straw being required to be left on the field. Another report by the RSB (2021) indicated that more than 60 million tonnes of lignocellulosic material (bagasse and straw) would be available for use. These estimations indicate that there is enough supply of LCM to produce the internal demand of SAF.

If the demand from all aviation companies to and from Brazil is considered, the total requirement for SAF is about 3 to 5 times the amount to supply only the national companies (by comparing Figure VI-11.a and c). Consequently, the amount of biomass required also increases proportionally. Considering only the straw available for use, the demand of this material would only be insufficient if Scenario 4 was adopted. However, the amount of LCM considered for this comparison is only the straw available on the Center-South region of Brazil (SOUZA et al., 2021), and with the supply of surplus bagasse from sugarcane mills would help meet this demand.

One important point to take into account is that these demands were calculated based on projections from 2018. The past couple of years has seen a decrease of jet fuel consumption due to the global crisis created by the COVID-19 pandemic. Figure VI-12 presents the historic variation of total demand for jet fuel (kerosene) for the Brazilian market, and it is clear that 2020 brought a sharp decrease in consumption of this fuel. It is still not clear how this oscillation will reflect on the goals of CORSIA: since the baseline is defined as the average of emissions from 2019 and 2020, the reduction of emissions from the past years should lead to a decrease of the CORSIA baseline, compared to the non-COVID-19 scenario (ICAO, 2022).

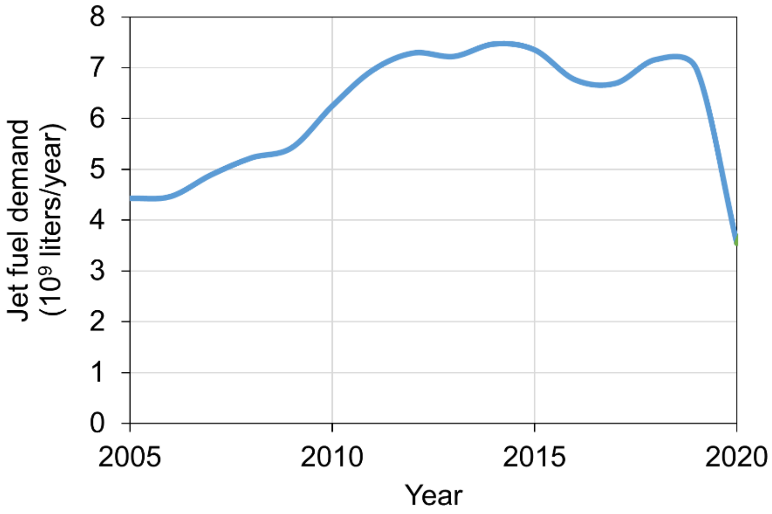

Figure VI-12 - Historical demand of jet fuel in Brazil (source:(ANP, 2022)*)*

Nonetheless, the projections from Figure VI-11 considered only the compulsory goals from CORSIA for the international flight sector, and other goals could be considered for the present analysis. For example, the most recent roadmap published by IEA (2021) raises some concerns about the current environmental scenario and the necessary actions to combat climate change. In order to mitigate emissions and minimize impacts, this report proposes some guidelines, among which is the aim to substitute at least 50% of aviation fuels to a clean alternative. With this more optimistic objective, it is possible to determine if the present route (GFT) has the potential to supply this demand.

With the historic values for jet fuel consumption for the Brazilian market (Figure VI-12), and considering a growth in demand of 2.3% per year (COELHO, 2019) it is possible to project a total demand of around 5.5 billion liters of jet fuel in 2040 (around 0.4 10^9 GJ of jet fuel/year). This estimation considers the growth from 2019, excluding the years of pandemic in order to avoid underestimating the consumption of fuels. To supply 50% of this consumption with SAF through Scenario1 would require around 60 M tonnes of dry LCM per year, while for the other three scenarios around 50 M tonnes of biomass would be required per year.

The requirement of biomass production to attend the substitution of 50% of the jet fuel consumption by 2040 with SAF from GFT routes is elevated, if compared to the demands from CORSIA alone. However, considering that the Center-South region alone produced around 50 Mtonnes of straw in 2018/2019 (SOUZA et al., 2021), it is safe to assume that it would be possible to meet this demand by adding the production of from other regions, the possible commercialization of surplus bagasse from sugarcane mills, and also considering the expansion of the sector.

Overall, these scenarios have the potential to provide SAF for the Brazilian market for the projected future, in terms of available biomass and fuel yield. It is also important to highlight that the fuel produced through these routes meet the requirement of being “drop-in”, since the aviation industry requires substitutes with equal performance characteristics of fossil fuel (BOEING et al., 2013).

The main hindrance for the implementation of these routes is the investment costs, as pointed out throughout this study, particularly for decentralized scenarios. The implementation of an integrated GFT-1G mill unit is economically attractive, while a standalone GFT unit processing bagasse and straw presents good environmental performance and, under favorable conditions with sufficient incentives, is also able to be economically feasible. Since the GFT route is also one of the only available and approved routes to obtain SAF (IRENA, 2017; SOONE, 2022), it is essential that investors and decision makers strive to help make these processes more feasible. The implementation of other routes – such as the Alcohol-to-Jet (ATJ) and Hydroprocessed Ester and Fatty Acids (HEFA) could even help and share the burden from the demand for SAF. Other sources of biomass could also be considered on the GFT processes, such as wood residues with a yearly availability of over 20 Mtonnes (RSB, 2021).

Chapter VII - Conclusion and future works

The use of the gasification of lignocellulosic biomasses followed by Fischer-Tropsch synthesis is a promising route to produce sustainable aviation fuel to help change the energy production and consumption to a cleaner and more environmental friendly scenario. According to the literature review for the present study, some of the main setbacks to the implementation of these processes were identified, and the high investment costs and problems with biomass supply are among the most important obstacles. The present study was successfully able to evaluate different configurations of implementing the GFT route into the Brazilian scenario. By developing simulation in Aspen Plus of the different industrial processes – fast pyrolysis, gasification and Fishcer-Tropsch synthesis – together with agricultural and logistic simulations it was possible to evaluate and compare these different options.

The integration of this thermochemical route with a first-generation ethanol distillery can utilize the well-stablished infrastructure and production chain of the Brazilian sugarcane sector, thus compensating both the high production costs of SAF and minimizing supply chain costs. This integrated scenario produced by far the best results from the evaluated configurations and is a solid benchmark for other renewable fuels productions processes.

The production of SAF through a Standalone GFT plant processing sugarcane bagasse and straw showed promising results: given a favorable scenario, or even with enough governmental aid and subsides, this configuration could achieve economic feasibility. Given the potential for GHG emission mitigation, this route has the most potential to help achieving the goals from different agreements and policies, such as the CORSIA. However, these favorable results are dependent of the GFT unit being built near the biomass production clusters, with the increasing distances having a harmful effect on the operational costs.

The results obtained from the scenarios with sugarcane residues have shown that the sugarcane sector is indeed a viable selection for the feedstock supplying option. The use of a decentralized production chain is another possibility to prevent making SAF production more expensive due to increased feedstocks costs from expenses with transportation. The present study considered the use of Fast pyrolysis units distributed near biomass production sites, thus obtaining an energetic dense intermediate (bio-oil) to be processed into more distant GFT units. In fact, this decentralized configuration leads to 60% fewer expenses with feedstock transportation than from a standalone biomass GFT plant. However, the investment costs with the additional process (FP) adds to the total costs and, consequently, the bio-oil becomes a more expensive alternative compared to solid biomass. With this, the decentralized option with bio-oil is a less attractive option for feedstock supply to the GFT route than from raw solid biomass. Bio-oil gasification is only competitive with the direct gasification for very long distances (above 1000 km), which is far beyond the figures observed in the Brazilian sugarcane industry.

Even though some of the proposed routes are yet to be economically attractive, all of them can meet the demands for GHG mitigation. All of the studied configurations represent significant reductions of GHG emissions from the fossil kerosene production and use. Moreover, the GFT route could be able to supply the required demand to substitute 50% of the total demand of jet fuel by 2040 considering the production of biomass residues from the country.

With the results obtained from the present study, a promising landscape unfolds: the production of SAF from GFT route can be economically viable while also achieving the required environmental goals, be it from the integration with 1G mills, or by developing a chain of production near biomass production sites with sufficient subsides. Further studies should aim to expand the results from this thesis.

Different technological options could be considered for the thermochemical conversion processes, such as equipment, and operational conditions. Variations to the gasification and Fischer-Tropsch reaction should be further studied to increase the carbon conversion and improve the efficiency of this route. An overall heat integration of the process through the Pinch analysis could also shed light on the possible improvements for this process, by lowering its energy consumption, for instance. Another interesting option to be assessed in further studies is the possible integration of SAF production with a crude-oil refinery. This would rely on the existing infrastructure to upgrade the syncrude, while also serving as an intermediate scenario between the current fossil-focused production and the biofuel production chain.

Besides changes to the main industrial process, the logistic aspects should also be further addressed. Firstly, the inclusion of other biomasses into the analysis would supply a wider perspective for the feedstock availability, thus leading to both larger production volumes as well as changing the logistic configuration around the biofuel plants. By also improving this type of analysis, a better understanding of the influence of plant decentralization would be possible . Georeferenced data with GIS tools is a manner to achieve more realistic results, and thus have a better representation of the actual Brazilian biomass production supply chain. Other decentralization options are also interesting, such as transporting bio-oil through ducts systems, or even the study of other densification processes such as torrefaction. These different options for future studies would help validate the current results, or even point out to new solutions for SAF production from thermochemical routes in the country.

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Annex A - Supplementary Material (Chapter III)

i. - Simulation description

The process of simulation and evaluation of the proposed route used the Virtual Sugarcane Biorefinery – VSB [1]. The VSB is a tool that integrates different computational platforms such as Aspen Plus®, SimaPro®, and electronic spreadsheets for the technical, economic, environmental, and social analyses. This tool allows the decision-making process by considering the agricultural technology, passing through the industrial processes, and reaching up to the logistics of use and distribution of the biofuel. This platform, developed by LNBR, is mainly utilized to evaluate the sugarcane sector but can also be adapted to assess different biomasses and industrial processes. This platform already contains a detailed representation of the sugar mill industrial process.

Mass and energy balances of the industrial phase of the integrated biorefinery were obtained from the Aspen Plus® process simulator version 8.6 (AspenTech, Bedford, MA, USA). To obtain an appropriate representation of the BtL plant and sugarcane biorefinery in the simulation, the main components and streams must be correctly described. The main components that are not present in the AspenPlus are the biomasses. Table A. 1 presents the proprieties considered for the lignocellulosic materials (bagasse + straw). Other components were obtained from the already existing VSB simulation framework. Table A. 2 present some of the more complex components that had to be simulated with a simpler component. For example, the different hydrocarbons product from the FT synthesis is represented by linear chain hydrocarbons.

Table A. 1 - Characterization of the lignocellulosic material (reference: VSB [1]*)*

	wt. % (d.b)
Proximate analysis	
Fixed carbon	16.79
Volatile matter	80.06
Ash	3.15
Ultimate analysis	
Ash	3.15
Carbon	46.69
Hydrogen	5.72
Nitrogen	0.32
Chlorine	0.04

Sulfur	0.05
Oxygen	44.03

Table A. 2 - Model components for the simulation of more complex components

Component	Model component	Formula	Reference
Minerals	Potassium-oxide	K2O	VSB [1]
Organic acids	Trans-aconitic-acid	C6H6O6	VSB [1]
Salts	Potassium-chloride	KCL	VSB [1]
Soil	Silicon-dioxide	SIO2	VSB [1]
C5	N-pentane	C5H12-1	[2]
C6	N-hexane	C6H14-1	[2]
C7	N-heptane	C7H16-1	[2]
C8	N-octane	C8H18-1	[2]
C9	N-nonane	C9H20-1	[2]
C10	N-decane	C10H22-1	[2]
C11	N-undecane	C11H24	[2]
C12	N-dodecane	C12H26	[2]
C13	N-tridecane	C13H28	[2]
C14	N-tetradecane	C14H30	[2]
C15	N-pentadecane	C15H32	[2]
C16	N-hexadecane	C16H34	[2]
C17	N-heptadecane	C17H36	[2]
C18	N-octadecane	C18H38	[2]
C19	N-nonadecane	C19H40	[2]
C20	N-eicosane	C20H42	[2]
C21	N-heneicosane	C21H44	[2]
C22	N-docosane	C22H46	[2]
C23	N-tricosane	C23H48	[2]
C24	N-tetracosane	C24H50	[2]
C25	N-pentacosane	C25H52	[2]
Waxes	N-triacontane	C30H62	[2]
MDEA	Methyl-diethanolamine	C5H13NO2	[3]
MDEA+	Mdea+	C5H14NO2+	[3]
Tar	Naphthalene	C10H8	[4]

The simulation was conceived for the thermochemical process integrated into a sugarcane mill. Figure A. 1 presents the overview of the simulation flowchart. Sugarcane stalks are retrieved from the field are destined to the preparation/extraction stage of the mill. The juice is destined to the distillery (where ethanol is produced) and bagasse is sent to the thermochemical process, with some fraction diverted to the distillery. Sugarcane straw left on the field is collected in the form of bales and sent directly to the BtL process. It is important to highlight that only the industrial process is contemplated in this simulation. The mill simulation is already established into the VSB framework and is detailed elsewhere [1]. The results for the mill are presented for the season period (200 days/year) so the streams of bagasse and straw are corrected to consider the whole period (330 days/year). Electricity and steam (2.5 bar) demands were calculated from the VSB framework and are dependent on the mill capacity.

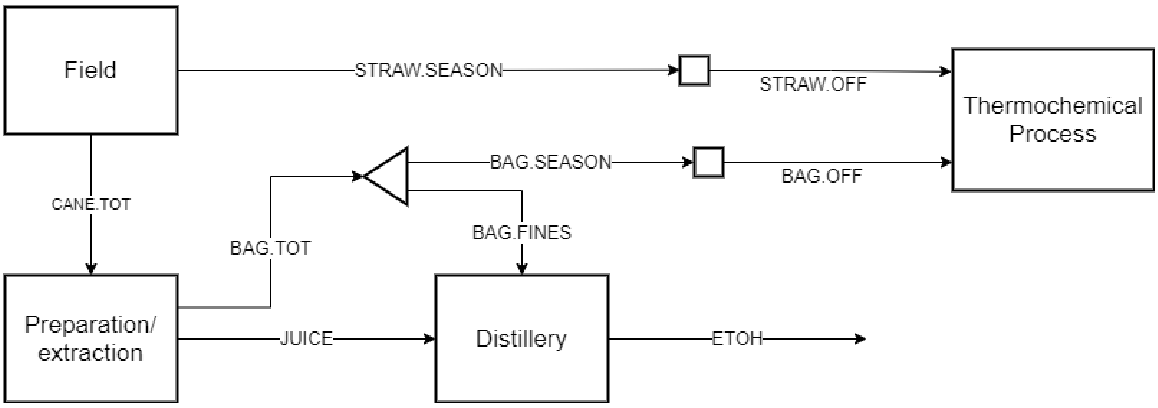

Figure A. 1 - Overall flowchart of the integrated plant

i.i. - - Preprocessing

The first step of the BtL process is the preprocessing of the LCM (Figure A. 2). The baled straw is chopped and sieved, and the resulting stream, together with the bagasse is dried to 10 wt.% moisture. Initially, the straw contains approximately 20-30% moisture, while for the bagasse this content is around 50%. The main consumption of this step is the electricity consumed on the sieves and chopper (total of 3.73 $kWh/ton_{straw\ d.b.}$) and the heat demand on the dryer (1.5 $MJ/kg_{evaporated\ water}$).

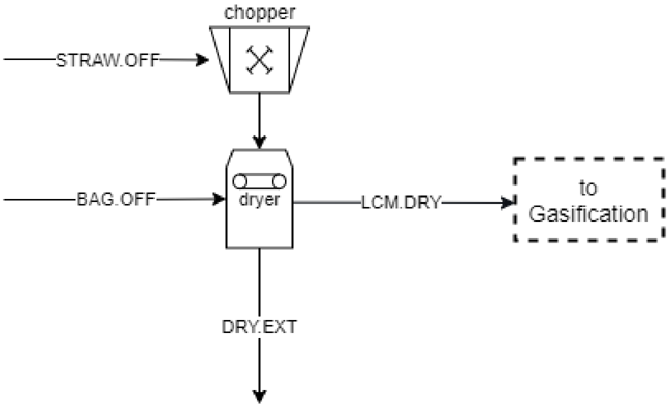

Figure A. 2 - Flowchart of the preprocessing of the lignocellulosic material

i.ii. - Gasification

Figure A. 3 presents the simplified flowchart of the gasification step. It was considered a low-pressure indirectly-heated circulating fluidized bed gasifier operating with steam (2.5 bar) at a ratio of 0.4 ton of steam per ton of dry biomass. The gasification simulation considered the correlations obtained by Bain et al [5] from the Battelle Columbus Laboratory (BCL). These correlations assume the form from Eq. A.01 dependent on the temperature (°F). Table A. 3 shows the values for each parameter. The temperature considered in the simulation was the equilibrium temperature obtained by Dutta et al. [6] (gasifier at 870 °C and combustor at 980 °C):

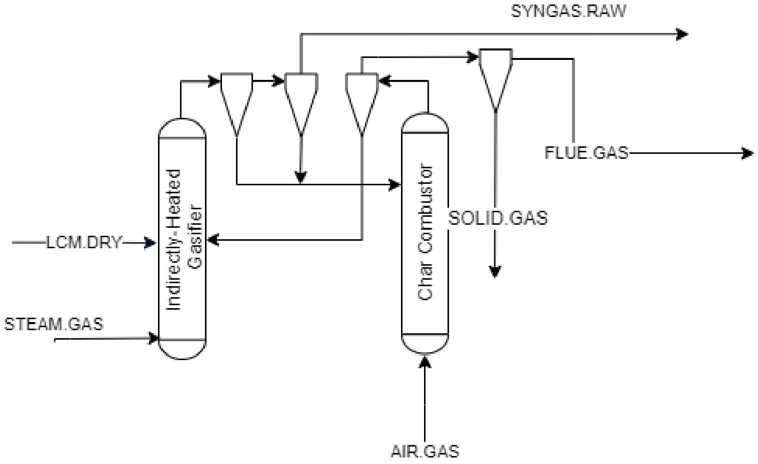

Figure A. 3 - Flowchart of the gasification process

$$Y = a + b.T + c.T^2 \quad \text{Eq. A.01}$$

Table A. 3 - Correlation parameters for gasification yields calculations [5]

Variable (Y)	**a**	**b**	**c**	**Units^b**
Dry syngas (mass)	0.1555	-0.0002206	0.000000376	lb/lb dry biomass
CO	133.4600	-0.1029	0.000028792	mole % dry gas
CO_2	-9.5251	0.037889	-0.000014927	mole % dry gas
CH_4	-13.8200	0.044179	-0.000016167	mole % dry gas
C_2H_4	-38.2580	0.058435	-0.000019868	mole % dry gas
C_2H_6	11.1140	-0.011667	0.000003064	mole % dry gas
H_2	17.9960	-0.026448	0.00001893	mole % dry gas
C_2H_2	-4.3114	0.0054499	-0.000001561	mole % dry gas
Tar ($C_{10}H_8$)	0.045494	-0.000019759	-	lb/lb dry biomass
Water conversion	0.2896	-0.00089048	0.00000043384	%

The produced amount of syngas as well as the quantities of each component are calculated from these correlations. This allows us to estimate the flow of each component on the resulting syngas. With the total flow of carbon present on the biomass and the carbon present in the syngas, the residual carbon is attached to the char. The same reasoning allows us to calculate the oxygen atomic content on the char.

8.3% of the sulfur and 6.6% of the nitrogen present on the biomass are transferred to the char [6]. The remaining atoms of these components are present in the form of H_2S and NH_3 in the syngas. All the chlorine is assumed to be set as HCl in syngas. Through mass balance, the content of hydrogen on the char is calculated. All ash is considered to be part of char. Further elaboration of the calculations can be found on Bressanin et al [7].

99.99% of the solid in the syngas are separated and sent to the combustor. 99% of the olivine from the combustor is separated from flue gas and recycled to the gasifier. Fresh olivine is added at a rate of 27 kg/kg of dry biomass [6]. The flue gas from the combustor is sent to heat integration to generate steam.

i.iii. - Syngas cleaning

The first step of the cleanup process (Figure A. 4) is the reforming, where methane, tars, and other light hydrocarbons are converted to CO and H_2, and NH_3 becomes N_2 and H_2. Table A. 4 presents the reactions considered for this stage, and the respective conversions considered [2,6,8]. Besides these reactions, it was also considered that the reactor also promotes Water-gas-shift reaction (Eq. A.02). Steam is added to the reactor to shift this equilibrium and correct the H_2/CO molar ratio to 2.1 at the entrance of the FT reactor.

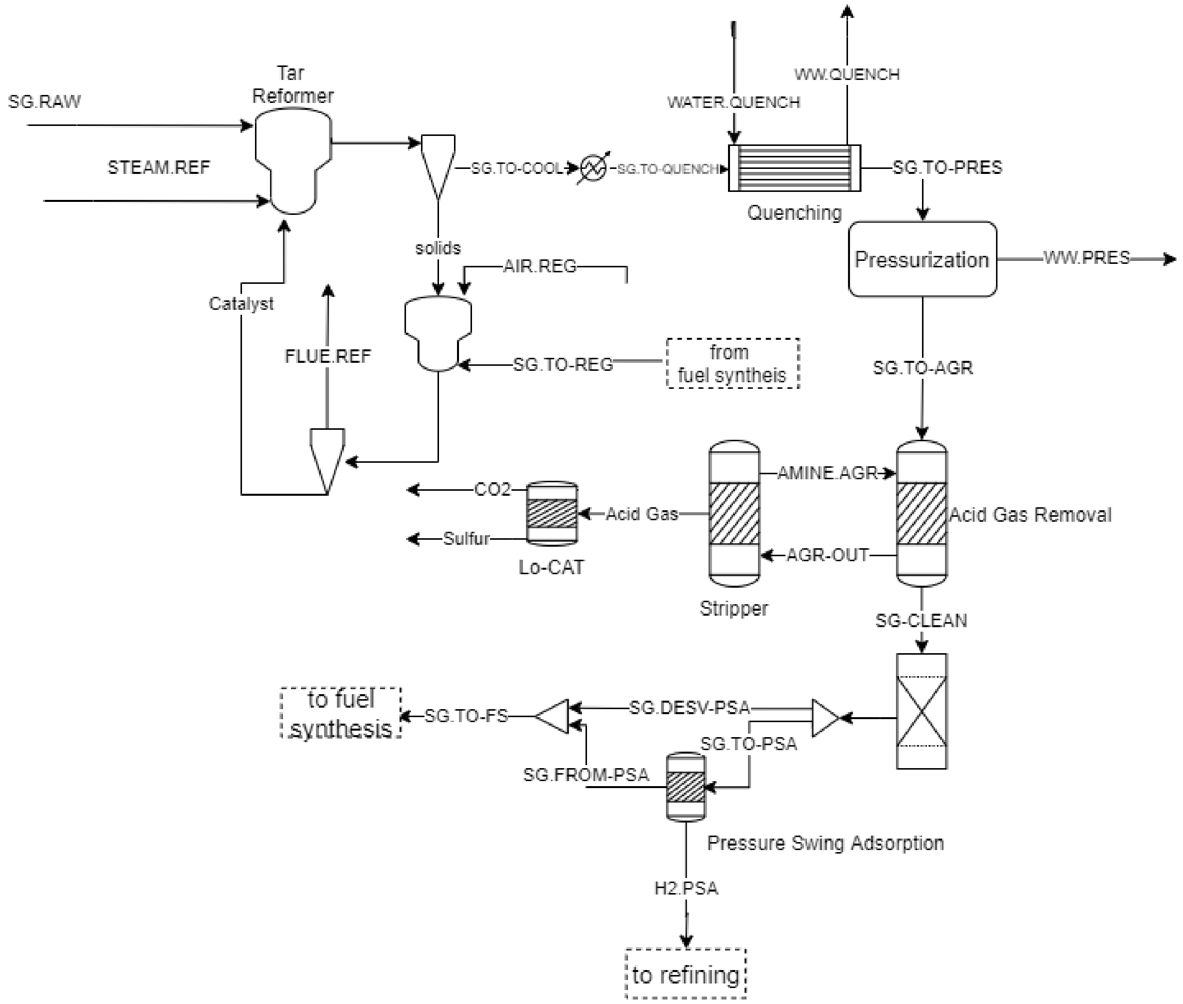

Figure A. 4 - Flowchart for the syngas cleanup processes

Table A. 4 - Reactions and conversions for the reforming process

Reaction	Conversion	Component
$TAR + 10\ H_2O \rightarrow 10\ CO + 14\ H_2$	0.99	TAR ($C_{10}H_8$)
$CH_4 + H_2O \rightarrow CO + 3\ H_2$	0.8	CH_4
$C_2H_4 + 2\ H_2O \rightarrow 2\ CO + 4\ H_2$	0.9	C_2H_4
$2\ NH_3 \rightarrow N_2 + 3\ H_2$	0.9	NH_3
$C_2H_6 + 2\ H2O \rightarrow 2\ CO + 5\ H_2$	0.9	C_2H_6

$$CO + H_2O \leftrightarrow CO_2 + H_2 \qquad \text{Eq. A.02}$$

The reforming section also counts with a catalyst regenerator that combusts the deposits from the catalyst particles. This regenerates the activity and supplies heat to the reforming reactions. Air is fed with 20% excess to the regenerator, and some unconverted syngas from the fuel synthesis stage is also supplied to help meet the heat demand. A two-stage cyclone separates the catalyst, and the combustion flue gases are used in heat integration. Around 0.03 kg of catalyst per ton of gas fed to the reformer is considered as make-up to replace the cyclones losses [7].

After reforming the syngas are cooled and sent to a scrubbing system. The first heat exchanger cools the syngas to around 60°C, and the heat is utilized to heat integration and steam generation. The scrubbing system works with a flow rate of 1 liter of water per m^3 of gas. Around 5 kg of fresh makeup, water per ton of circulating water is required [6] and the electricity requirement of this process is assumed to be 0.1 kWh per ton of syngas [9].

The pressurization of the syngas occurs on a 5-stage centrifugal compressor with knock-out drums up to around 25 bar. The calculated energy consumption is around 0.19 kWh/m^3 of syngas.

In this study, it is considered the use of a 30 %wt. methyl diethanolamine solution for the Acid-Gas-Removal (AGR) process. The process was simulated by considering the reactions between the amine and H_2S/CO_2. Table A. 5 shows the considered reactions and the conversion for each component [3,9]. It was considered that 0.01% of the circulating amine is lost and must be made up for. Make-up water is assumed to be enough to maintain the concentration of amine. A flash separator and a stripper column regenerate the amine removing the acid gas, and the lean amine is cooled and cycled back to the absorber. This process consumes 4 bar steam (at a rate of around 3620 MJ per ton of acid gas), around 1.06 kWh of electricity per mass of circulating solvent, and 32.2 tons of cooling water supplied per ton of syngas inlet [9]. A LO-CAT® unit removes the sulfur from the acid gas, and it is assumed that 0.08 t LO-CAT chemical is necessary per ton of sulfur, together with 4.7% of makeup water in sour gas, 0.28 kg of steam per kmol of acid gas, and electricity consumption of 0.5 kWh electricity per kmol of acid gas [9].

Table A. 5 - Reactions and conversions for the acid gas removal process

Reaction	Conversion	Component
$\mathbf{MDEA + H_2S \rightarrow MDEA^+ + HS^-}$	0.99	H2S
$\mathbf{MDEA + CO_2 + H_2O \rightarrow MDEA^+ + HCO_3^-}$	0.9	CO2

A ZnO bed is used to remove even more sulfur from the syngas to contents below 50 ppb [9]. This process was not directly simulated, but the consumption of fresh catalysts was considered for the analysis. The ZnO is replaced in a period of 1 year, requiring a volume of 48.5 m^3 of catalyst per kg of H_2S remaining on the syngas [9].

A PSA unit deviates part of the hydrogen present on the syngas. This hydrogen is necessary for the hydroprocessing process on the fuel synthesis step. An efficiency of 85% of the removal of hydrogen is assumed, producing a pure H_2 stream [2].

i.iv. - Fuel synthesis

FT synthesis (Figure A. 5) was conducted on a tubular fixed bed reactor, with cobalt catalyst and inlet pressure and temperature of 25 bar and 200 °C. This process produces several hydrocarbons with variable chain lengths, and these products can be described by the Anderson-Schulz-Flory (ASF) distribution. The yield of each hydrocarbon (X_n – Eq 03) is determined by the chain growth probability (α) model, and dependent on the length of the chain (n – number of carbons) [10], as seen on Eq. A.04. The calculation of the flow of each hydrocarbon chain (C1 until C25+) follows the detailed steps described by Swanson et al [2]

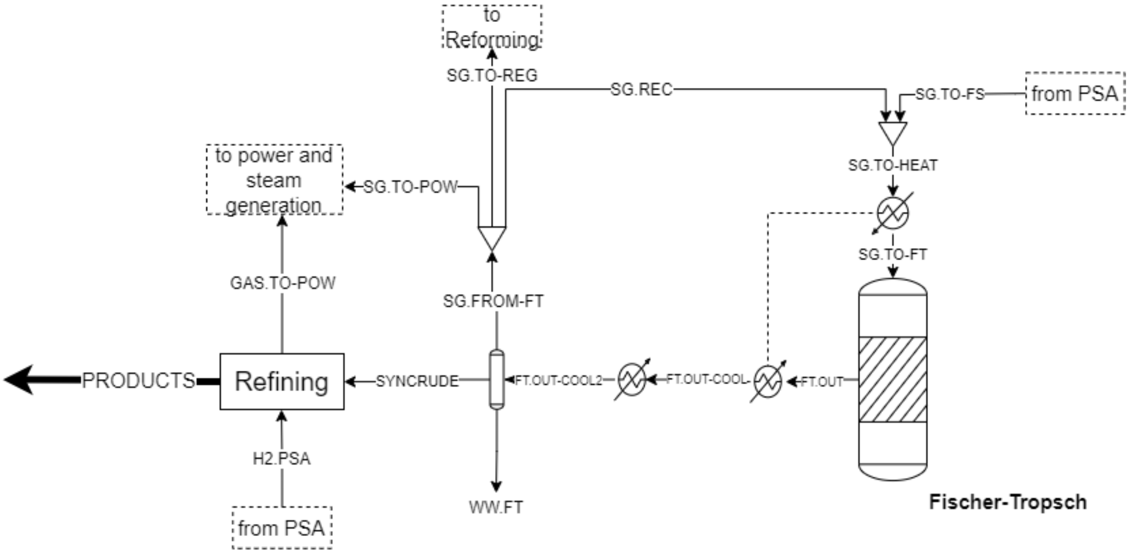

Figure A. 5 - Flowchart for the fuel synthesis processes

$$\alpha = \left(\frac{0.2332\, y_{CO}}{y_{CO} + y_{H_2}} + 0.6330\right).[1 - 0.0039(T - 533)] \qquad \text{Eq. A.03}$$

$$X_n = \alpha^{(n-1)}.(1 - \alpha) \qquad \text{Eq. A.04}$$

With y_{co} and y_{H2} the molar fraction of CO and H_2, respectively, and T the temperature (K)

The FT reactions are highly exothermic, and the heat produced on the reactor is utilized to generate steam for the power generation of the plant.

Part of the unconverted syngas is sent to power generation and the regenerator (tar reforming), while the rest is recycled back to the reactor. A per-pass carbon monoxide conversion of 40% [2] is considered.

The liquid products from the FT synthesis are separated into a water stream, and an organic liquid stream, composed of the different hydrocarbons. For the simulation this process of separation was simplified, consisting of a one-stage separator block. For actual applications, during an industrial process, this step would involve at least a two-stage separation to avoid problems such as blockage by wax formation. However, the process can be adequately represented by the current simplification.

The hydrocarbon stream is sent to the refining/hydroprocessing section. The simulation of this stage was done considering the yields proposed by Klerk [11] for a refinery design of a Low-Temperature-Fischer-Tropsch process maximizing the production of kerosene (jetfuel) with co-production of green gasoline. The gases produced are added to the unreacted syngas from the FT reactor destined for energy generation. The composition of the resulting products is shown in Table A. 6. The electricity demand of this process is 0.125 MW/t FT liquids per hour [2], and around 0.43 MWh of energy per ton of FT liquids processed is released to cooling water.

Table A. 6 - Product yields for the hydroprocessing unit [11]

Product	**Mass composition %**
Gasoline	19.6
Jet fuel	57.0
Combustible gases (C_2H_6)	7.4
LPG (C_3H_8)	11.4
Others	4.6

i.v. - Power and steam generation

The heat integration and power generation of the plant consider the following (Figure A. 6 and Figure A. 7):

- Part of the unconverted syngas/gaseous products are destined to supply heat to the tar reforming catalyst regenerator;
- Deviation of part of the unconverted syngas and the gaseous products to a gas turbine. Excess air is calculated to achieve a temperature of around 610 °C at the inlet of the turbine. This turbine operates with an inlet pressure of 20 bar, with a pressure ratio of 0.05;
- The exhaust from the gas turbine is used to produce superheated steam (90 bar, 520 °C).
- Additional superheated steam (90 bar, 520 °C) from the heat from the cooling of the syngas (before quenching) and the heat of the flue gas from the regenerator (tar reforming) and combustor (gasification);

- 20 bar steam produced from the heat removed from the FT reactor;
- A back-pressure steam turbine with an inlet pressure of 90 bar drops the pressure initially to 20 bar. This outlet is added to the steam produced from the heat integration of the FT reactor and directed to a condensing extraction turbine. Some amount of 4 bar steam is extracted to supply the AGR demands, and 2.5 bar is extracted to meet the demands from the mill, gasification, reforming, and LOCAT processes.
- Electricity produced from these turbines (gas and steam turbines) supplies all the power demand of the plant.

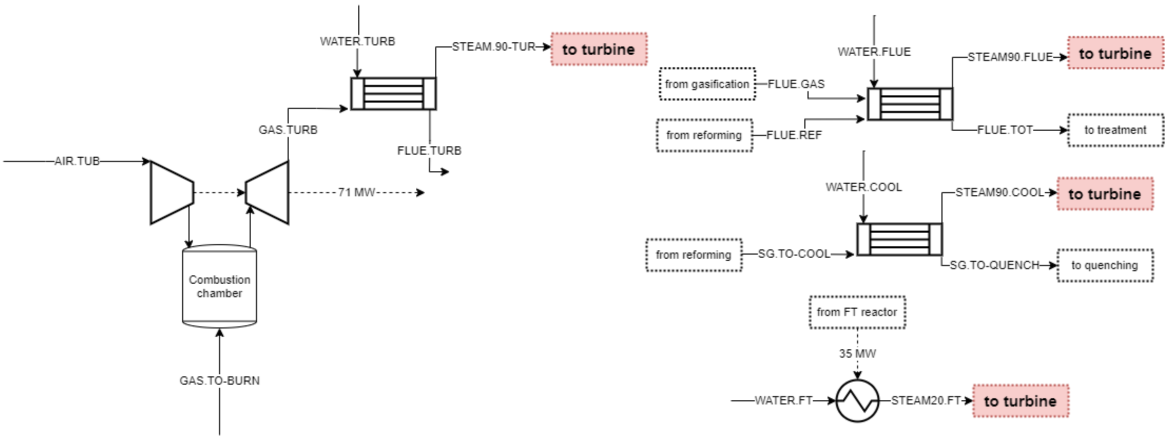

Figure A. 6 - Flowchart for the heat integration/steam generation

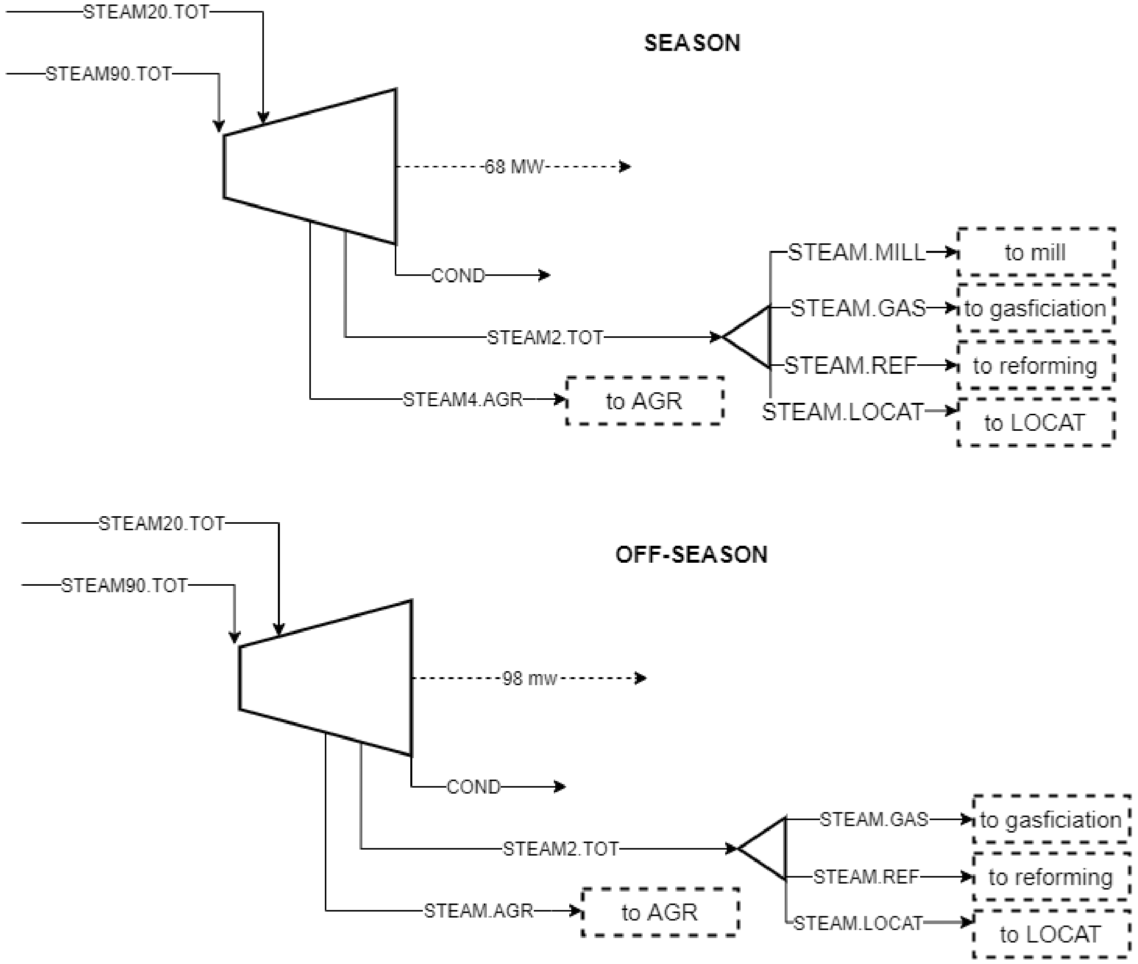

Figure A. 7 - Flowchart for the electricity production/steam generation

ii. - Mass and Energy Balances

According to the nomenclatures presented from Figure A. 2 to Figure A. 7, the following tables present the mass and energy balances for each stream.

Table A. 7 - Mass and energy Balance: Sugarcane Mill

	Units	**CANE.TOT**	**JUICE**	**ETOH**	**BAG.TOT**	**BAG.FINES**	**BAG.SEASON**	**BAG.OFF**	**STRAW.SEASON**	**STRAW.OFF**
Temperature	C	25	29	81	29	29	29	29	25	25
Pressure	bar	1.013	1.013	1.16	1.013	1.013	1.013	1.013	1.013	1.013
Enthalpy Flow	MW	-3008	-3380	-109	-704	-15	-689	-417	-168	-102
Mass Flows	kg/hr	851574	854152	60010	242374	5109	237265	143797	72855	44155
CO2	kg/hr	0	0	1	0	0	0	0	0	0
Ethanol	kg/hr	0	0	55794	0	0	0	0	0	0
Glucose	kg/hr	4995	4792	0	203	4	199	121	134	81
Glycerol	kg/hr	0	0	0	0	0	0	0	0	0
H2O	kg/hr	592672	716335	4214	121289	2557	118732	71959	21711	13158
H3PO4	kg/hr	251	238	0	13	0	13	8	13	8
Isobutanol	kg/hr	0	0	0	0	0	0	0	0	0
Minerals	kg/hr	1658	1358	0	300	6	294	178	8	5
Organic acids	kg/hr	4693	4477	0	216	5	211	128	296	179
Salts	kg/hr	13327	10955	0	2373	50	2322	1408	1299	787
Sucrose	kg/hr	116546	111800	0	4746	100	4646	2816	3100	1879
Acetate	kg/hr	2976	42	0	2934	62	2872	1741	1353	820
Cellulose	kg/hr	53121	750	0	52371	1104	51267	31071	19043	11541
Lignin	kg/hr	28810	407	0	28403	599	27805	16851	12071	7316
Soil	kg/hr	3500	2589	0	911	19	891	540	629	381
Xylan	kg/hr	29024	410	0	28614	603	28011	16976	13197	7998

Table A. 8 - Mass and Energy Balance: Preprocessing

	Units	**BAG.OFF**	**STRAW.OFF**	**DRY.EXT**	**LCM.DRY**
Temperature	C	25	25	120	120
Pressure	bar	1.2	1.2	1.2	1.2
Enthalpy Flow	MW	-430	-107	-271	-206
Mass Flows	kg/hr	143782	44150	73684	114249
H2O	kg/hr	71952	13157	73684	11425
Biomass	kg/hr	71831	30993	0	102824
Biomass ultimate analysis					
Ash	kg/hr	2263	976	-	3239
Carbon	kg/hr	33538	14471	-	48008
Hydrogen	kg/hr	4109	1773	-	5882
Nitrogen	kg/hr	230	99	-	329
Chlorine	kg/hr	29	12	-	41
Sulfur	kg/hr	36	15	-	51
Oxygen	kg/hr	31627	13646	-	45273

Table A. 9 - Mass and Energy Balance: Gasification

	Units	**STEAM.GAS**	**AIR.GAS**	**SOLID.GAS**	**FLUE.GAS**	**SYNGAS.RAW**
Temperature	C	310	450	987	987	870
Pressure	bar	2.5	1.32	1.32	1.32	1.3
Enthalpy Flow	MW	-147	24	0.2	-104	-240
Mass Flows	kg/hr	41129	196364	3239	219527	128977
CH4	kg/hr	0	0	0	0	8579
CO2	kg/hr	0	0	0	52420	19601
H2O	kg/hr	41129	0	0	11399	52539
N2	kg/hr	0	150628	0	150649	0
O2	kg/hr	0	45737	0	5008	0
SO2	kg/hr	0	0	0	10	0
H2	kg/hr	0	0	0	0	1675
CO	kg/hr	0	0	0	0	41135
CL2	kg/hr	0	0	0	41	41
NH3	kg/hr	0	0	0	0	374
H2S	kg/hr	0	0	0	0	50
C2H6	kg/hr	0	0	0	0	306
C2H4	kg/hr	0	0	0	0	4247
TAR (C10H8)	kg/hr	0	0	0	0	62
C2H2	kg/hr	0	0	0	0	370
ASH	kg/hr	0	0	3239	0	0

Table A. 10 - Mass and Energy Balance: Syngas cleaning

	Units	SYNGAS.RAW	STEAM.REF	SG.TO-REG	AIR.REG	FLUE.REF
Temperature	C	870	310	25	450	969
Pressure	bar	1.3	2.5	25.0	1.3	1.8
Enthalpy Flow	MW	-240	-77	-9	9	-43
Mass Flows	kg/hr	128977	21475	8699	75561	84261
CH_4	kg/hr	8579	0	456	0	0
CO_2	kg/hr	19601	0	899	0	13472
H_2O	kg/hr	52539	21475	0	0	9827
N_2	kg/hr	0	0	68	57962	58029
O_2	kg/hr	0	0	0	17600	2933
H_2	kg/hr	1675	0	841	0	0
CO	kg/hr	41135	0	5606	0	0
CL_2	kg/hr	41	0	0	0	0
NH_3	kg/hr	374	0	0	0	0
H_2S	kg/hr	50	0	0	0	0
C_2H_6	kg/hr	306	0	316	0	0
C_2H_4	kg/hr	4247	0	84	0	0
TAR ($C_{10}H_8$)	kg/hr	62	0	0	0	0
C3	kg/hr	0	0	142	0	0
C4	kg/hr	0	0	120	0	0
C5	kg/hr	0	0	19	0	0
C6	kg/hr	0	0	20	0	0
C7	kg/hr	0	0	10	0	0
C8	kg/hr	0	0	10	0	0
C9	kg/hr	0	0	10	0	0
C10	kg/hr	0	0	9	0	0
C11	kg/hr	0	0	4	0	0
C12	kg/hr	0	0	4	0	0
C13	kg/hr	0	0	4	0	0
C14	kg/hr	0	0	4	0	0
C15	kg/hr	0	0	4	0	0
C16	kg/hr	0	0	3	0	0
MDEA	kg/hr	0	0	0	0	0
MDEA+	kg/hr	0	0	0	0	0
HS^-	kg/hr	0	0	0	0	0
HCO_3^-	kg/hr	0	0	0	0	0
C_2H_2	kg/hr	370	0	67	0	0

Table A. 11 - Mass and Energy Balance: Syngas cleaning (cont)

	Units	**SG.TO-COOL**	**SG.TO-QUENCH**	**WATER.QUENCH**	**WW.QUENCH**
Temperature	C	910	54	25	44
Pressure	bar	1.8	1.8	1.3	1.3
Enthalpy Flow	MW	-274	-376	-450	-508
Mass Flows	kg/hr	150452	150452	102201	115944
CH4	kg/hr	1716	1716	0	0
CO2	kg/hr	45615	45615	0	0
H2O	kg/hr	50334	50334	102201	115926
N2	kg/hr	277	277	0	0
O2	kg/hr	0	0	0	0
H2	kg/hr	6717	6717	0	0
CO	kg/hr	44840	44840	0	0
CL2	kg/hr	41	41	0	0
NH3	kg/hr	37	37	0	15
H2S	kg/hr	50	50	0	2
C2H6	kg/hr	31	31	0	0
C2H4	kg/hr	425	425	0	0
TAR (C10H8)	kg/hr	1	1	0	0
C3	kg/hr	0	0	0	0
C4	kg/hr	0	0	0	0
C5	kg/hr	0	0	0	0
C6	kg/hr	0	0	0	0
C7	kg/hr	0	0	0	0
C8	kg/hr	0	0	0	0
C9	kg/hr	0	0	0	0
C10	kg/hr	0	0	0	0
C11	kg/hr	0	0	0	0
C12	kg/hr	0	0	0	0
C13	kg/hr	0	0	0	0
C14	kg/hr	0	0	0	0
C15	kg/hr	0	0	0	0
C16	kg/hr	0	0	0	0
MDEA	kg/hr	0	0	0	0
MDEA+	kg/hr	0	0	0	0
HS-	kg/hr	0	0	0	0
HCO3-	kg/hr	0	0	0	0
C2H2	kg/hr	370	370	0	0

Table A. 12 - Mass and Energy Balance: Syngas cleaning (cont)

	Units	**SG.TO-PRES**	**WW.PRES**	**SG.TO-AGR**	**AMINE.AGR**	**AGR-OUT**
Temperature	C	44	43	43	48	44
Pressure	bar	1.3	1.3	25.3	1.3	25.0
Enthalpy Flow	MW	-318	-160	-163	-449	-265
Mass Flows	kg/hr	136709	36629	100080	195093	238356
CH4	kg/hr	1716	3	1713	0	90
CO2	kg/hr	45615	327	45288	0	935
H2O	kg/hr	36608	36253	356	73519	56985
N2	kg/hr	277	0	276	0	6
O2	kg/hr	0	0	0	0	0
H2	kg/hr	6717	0	6717	0	12
CO	kg/hr	44840	29	44810	0	1036
CL2	kg/hr	41	2	39	0	26
NH3	kg/hr	22	6	16	0	14
H2S	kg/hr	47	1	46	0	0
C2H6	kg/hr	31	0	30	0	9
C2H4	kg/hr	425	3	422	0	86
TAR (C10H8)	kg/hr	1	1	0	0	0
C3	kg/hr	0	0	0	0	0
C4	kg/hr	0	0	0	0	0
C5	kg/hr	0	0	0	0	0
C6	kg/hr	0	0	0	0	0
C7	kg/hr	0	0	0	0	0
C8	kg/hr	0	0	0	0	0
C9	kg/hr	0	0	0	0	0
C10	kg/hr	0	0	0	0	0
C11	kg/hr	0	0	0	0	0
C12	kg/hr	0	0	0	0	0
C13	kg/hr	0	0	0	0	0
C14	kg/hr	0	0	0	0	0
C15	kg/hr	0	0	0	0	0
C16	kg/hr	0	0	0	0	0
MDEA	kg/hr	0	0	0	121574	11052
MDEA+	kg/hr	0	0	0	0	111456
HS-	kg/hr	0	0	0	0	44
HCO3-	kg/hr	0	0	0	0	56511
C2H2	kg/hr	370	4	366	0	94

Table A. 13 - Mass and Energy Balance: Syngas cleaning (cont)

	Units	SG.CLEAN	SG.DESV-PSA	SG.TO-PSA	SG.FROM-PSA	SG.TO-FS	H2.PSA
Temperature	C	44	44	44	44	44	44
Pressure	bar	25.0	25.0	25.0	25.0	25.0	25.0
Enthalpy Flow	MW	-58	-57	-1	-1	-58	0.01
Mass Flows	kg/hr	56817	56120	697	624	56744	73
CH4	kg/hr	1623	1604	20	20	1623	0
CO2	kg/hr	3594	3550	44	44	3594	0
H2O	kg/hr	205	202	3	3	205	0
N2	kg/hr	270	267	3	3	270	0
O2	kg/hr	0	0	0	0	0	0
H2	kg/hr	6705	6623	82	12	6635	70
CO	kg/hr	43774	43237	537	537	43774	0
CL2	kg/hr	13	13	0	0	13	0
NH3	kg/hr	2	2	0	0	2	0
H2S	kg/hr	0	0	0	0	0	0
C2H6	kg/hr	21	21	0	0	21	0
C2H4	kg/hr	335	331	4	4	335	0
TAR (C10H8)	kg/hr	0	0	0	0	0	0
C3	kg/hr	0	0	0	0	0	0
C4	kg/hr	0	0	0	0	0	0
C5	kg/hr	0	0	0	0	0	0
C6	kg/hr	0	0	0	0	0	0
C7	kg/hr	0	0	0	0	0	0
C8	kg/hr	0	0	0	0	0	0
C9	kg/hr	0	0	0	0	0	0
C10	kg/hr	0	0	0	0	0	0
C11	kg/hr	0	0	0	0	0	0
C12	kg/hr	0	0	0	0	0	0
C13	kg/hr	0	0	0	0	0	0
C14	kg/hr	0	0	0	0	0	0
C15	kg/hr	0	0	0	0	0	0
C16	kg/hr	0	0	0	0	0	0
MDEA	kg/hr	0	0	0	0	0	0
MDEA+	kg/hr	0	0	0	0	0	0
HS-	kg/hr	0	0	0	0	0	0
HCO3-	kg/hr	0	0	0	0	0	0
C2H2	kg/hr	272	269	3	0	269	3

Table A. 14 - Mass and Energy Balance: Fuel Synthesis

	Units	**SG.TO-FS**	**SG.TO-HEAT**	**SG.TO-FT**	**FT.OUT**	**FT.OUT-COOL**
Temperature	C	44	40	200	200	122
Pressure	bar	25	25	25	25	25
Enthalpy Flow	MW	-58	-74	-65	-100	-108
Mass Flows	kg/hr	56744	71197	71197	71197	71197
CH4	kg/hr	1623	2404	2404	2602	2602
CO2	kg/hr	3594	5134	5134	5134	5134
H2O	kg/hr	205	205	205	13938	13938
N2	kg/hr	270	386	386	386	386
O2	kg/hr	0	0	0	0	0
SO2	kg/hr	0	0	0	0	0
H2	kg/hr	6635	8078	8078	4807	4807
CO	kg/hr	43774	53383	53383	32030	32030
CL2	kg/hr	13	13	13	13	13
NH3	kg/hr	2	2	2	2	2
H2S	kg/hr	0	0	0	0	0
C2H6	kg/hr	21	170	170	494	494
C2H4	kg/hr	335	479	479	479	479
C3	kg/hr	0	178	178	594	594
C4	kg/hr	0	205	205	684	684
C5	kg/hr	0	33	33	552	552
C6	kg/hr	0	35	35	576	576
C7	kg/hr	0	17	17	567	567
C8	kg/hr	0	17	17	565	565
C9	kg/hr	0	17	17	554	554
C10	kg/hr	0	16	16	537	537
C11	kg/hr	0	8	8	507	507
C12	kg/hr	0	7	7	483	483
C13	kg/hr	0	7	7	456	456
C14	kg/hr	0	6	6	429	429
C15	kg/hr	0	6	6	401	401
C16	kg/hr	0	6	6	373	373
C17	kg/hr	0	0	0	341	341
C18	kg/hr	0	0	0	315	315
C19	kg/hr	0	0	0	291	291
C20	kg/hr	0	0	0	267	267
C21	kg/hr	0	0	0	245	245
C22	kg/hr	0	0	0	224	224
C23	kg/hr	0	0	0	205	205
C24	kg/hr	0	0	0	186	186
C25	kg/hr	0	0	0	170	170
WAXES	kg/hr	0	0	0	1403	1403
MDEA	kg/hr	0	0	0	0	0
GASOLINE	kg/hr	0	0	0	0	0
JETFUEL	kg/hr	0	0	0	0	0
C2H2	kg/hr	269	384	384	384	384

Table A. 15 - Mass and Energy Balance: Fuel Synthesis (cont)

	Units	**FT.OUT-COOL2**	**WW.FT**	**SG.FROM-FT**	**SG.REC**	**SG.TO-REG**
Temperature	C	25	25	25	25	25
Pressure	bar	25	25	25	25	25
Enthalpy Flow	MW	-118	-61	-52	-15	-9
Mass Flows	kg/hr	71197	13954	48176	14453	8699
CH4	kg/hr	2602	0	2602	781	456
CO2	kg/hr	5134	0	5134	1540	899
H2O	kg/hr	13938	13938	0	0	0
N2	kg/hr	386	0	386	116	68
O2	kg/hr	0	0	0	0	0
SO2	kg/hr	0	0	0	0	0
H2	kg/hr	4807	0	4807	1442	841
CO	kg/hr	32030	0	32030	9609	5606
CL2	kg/hr	13	13	0	0	0
NH3	kg/hr	2	2	0	0	0
H2S	kg/hr	0	0	0	0	0
C2H6	kg/hr	494	0	494	148	316
C2H4	kg/hr	479	0	479	144	84
C3	kg/hr	594	0	594	178	142
C4	kg/hr	684	0	684	205	120
C5	kg/hr	552	0	110	33	19
C6	kg/hr	576	0	115	35	20
C7	kg/hr	567	0	57	17	10
C8	kg/hr	565	0	56	17	10
C9	kg/hr	554	0	55	17	10
C10	kg/hr	537	0	54	16	9
C11	kg/hr	507	0	25	8	4
C12	kg/hr	483	0	24	7	4
C13	kg/hr	456	0	23	7	4
C14	kg/hr	429	0	21	6	4
C15	kg/hr	401	0	20	6	4
C16	kg/hr	373	0	19	6	3
C17	kg/hr	341	0	0	0	0
C18	kg/hr	315	0	0	0	0
C19	kg/hr	291	0	0	0	0
C20	kg/hr	267	0	0	0	0
C21	kg/hr	245	0	0	0	0
C22	kg/hr	224	0	0	0	0
C23	kg/hr	205	0	0	0	0
C24	kg/hr	186	0	0	0	0
C25	kg/hr	170	0	0	0	0
WAXES	kg/hr	1403	0	0	0	0
MDEA	kg/hr	0	0	0	0	0
GASOLINE	kg/hr	0	0	0	0	0
JETFUEL	kg/hr	0	0	0	0	0
C2H2	kg/hr	384	0	384	115	67

Table A. 16 - Mass and Energy Balance: Fuel Synthesis (cont)

	Units	**SG.TO-POW**	**SYNCRUDE**	**H2.PSA**	**GAS.TO-POW**	**PRODUCTS**
Temperature	C	25	25	44	26	26
Pressure	bar	25	25	25	25	25
Enthalpy Flow	MW	-28	-5	0.01	-1	-5
Mass Flows	kg/hr	26093	9066	73	1068	8068
CH4	kg/hr	1366	0	0	0	0
CO2	kg/hr	2695	0	0	0	0
H2O	kg/hr	0	0	0	0	0
N2	kg/hr	203	0	0	0	0
O2	kg/hr	0	0	0	0	0
SO2	kg/hr	0	0	0	0	0
H2	kg/hr	2524	0	70	0	0
CO	kg/hr	16815	0	0	0	0
CL2	kg/hr	0	0	0	0	0
NH3	kg/hr	0	0	0	0	0
H2S	kg/hr	0	0	0	0	0
C2H6	kg/hr	947	0	0	916	0
C2H4	kg/hr	252	0	0	0	0
C3	kg/hr	426	0	0	152	0
C4	kg/hr	359	0	0	0	0
C5	kg/hr	58	442	0	0	0
C6	kg/hr	60	461	0	0	0
C7	kg/hr	30	510	0	0	0
C8	kg/hr	30	508	0	0	0
C9	kg/hr	29	498	0	0	0
C10	kg/hr	28	483	0	0	0
C11	kg/hr	13	482	0	0	0
C12	kg/hr	13	458	0	0	0
C13	kg/hr	12	433	0	0	0
C14	kg/hr	11	407	0	0	0
C15	kg/hr	11	381	0	0	0
C16	kg/hr	10	355	0	0	0
C17	kg/hr	0	341	0	0	0
C18	kg/hr	0	315	0	0	0
C19	kg/hr	0	291	0	0	0
C20	kg/hr	0	267	0	0	0
C21	kg/hr	0	245	0	0	0
C22	kg/hr	0	224	0	0	0
C23	kg/hr	0	205	0	0	0
C24	kg/hr	0	186	0	0	0
C25	kg/hr	0	170	0	0	0
WAXES	kg/hr	0	1403	0	0	0
MDEA	kg/hr	0	0	0	0	0
GASOLINE	kg/hr	0	0	0	0	2081
JETFUEL	kg/hr	0	0	0	0	5987
C2H2	kg/hr	202	0	3	0	0

Table A. 17 - Mass and Energy Balance: Steam and Power generation

	Units	**GAS.TO-BURN**	**AIR.TURB**	**GAS.TURB**	**WATER.TURB**	**STEAM.90-TUR**
Temperature	C	25	25	609.9998867	111	520
Pressure	bar	25	1.01325	1	1.5	90
Enthalpy Flow	MW	-28	-4.46E-15	-99	-471	-378
Mass Flows	kg/hr	26093	592051	618144	109510	109510
CH4	kg/hr	1366	0	0	0	0
CO2	kg/hr	2695	0	40406	0	0
H2O	kg/hr	0	0	29473	109510	109510
N2	kg/hr	203	454153	454355	0	0
O2	kg/hr	0	137899	93909	0	0
SO2	kg/hr	0	0	0	0	0
H2	kg/hr	2524	0	0	0	0
CO	kg/hr	16815	0	0	0	0
CL2	kg/hr	0	0	0	0	0
NH3	kg/hr	0	0	0	0	0
H2S	kg/hr	0	0	0	0	0
C2H6	kg/hr	947	0	0	0	0
C2H4	kg/hr	252	0	0	0	0
TAR (C10H8)	kg/hr	0	0	0	0	0
C3	kg/hr	426	0	0	0	0
C4	kg/hr	359	0	0	0	0
C5	kg/hr	58	0	0	0	0
C6	kg/hr	60	0	0	0	0
C7	kg/hr	30	0	0	0	0
C8	kg/hr	30	0	0	0	0
C9	kg/hr	29	0	0	0	0
C10	kg/hr	28	0	0	0	0
C11	kg/hr	13	0	0	0	0
C12	kg/hr	13	0	0	0	0
C13	kg/hr	12	0	0	0	0
C14	kg/hr	11	0	0	0	0
C15	kg/hr	11	0	0	0	0
C16	kg/hr	10	0	0	0	0
C2H2	kg/hr	202	0	0	0	0

Table A. 18 - Mass and Energy Balance: Steam and Power generation (cont)

	Units	FLUE.TURB	FLUE.GAS	FLUE.REF	FLUE.TOT	WATER.FLUE	STEAM90.FLUE	SG.TO-COOL	SG.TO-QUENCH	WATER.COOL	STEAM90.COOL	WATER.FT	STEAM20.FT
Temperature	C	130	987	969	130	111	520	910	54	111	520	110	330
Pressure	bar	1	1.32	1.77	1.32	1.5	90	1.77	1.77	1.5	90	1.5	20
Enthalpy Flow	MW	-191	-104	-43	-233	-442	-355	-274	-376	-353	-284	-204	-169
Mass Flows	kg/hr	618144	219527	84261	303787	102618	102618	150452	150452	82135	82135	47320	47320
CH_4	kg/hr	0	0	0	0	0	0	1716	1716	0	0	0	0
CO_2	kg/hr	40406	52420	13472	65892	0	0	45615	45615	0	0	0	0
H_2O	kg/hr	29473	11399	9827	21226	102618	102618	50334	50334	82135	82135	47320	47320
N_2	kg/hr	454355	150649	58029	208679	0	0	277	277	0	0	0	0
O_2	kg/hr	93909	5008	2933	7941	0	0	0	0	0	0	0	0
SO_2	kg/hr	0	10	0	10	0	0	0	0	0	0	0	0
H_2	kg/hr	0	0	0	0	0	0	6717	6717	0	0	0	0
CO	kg/hr	0	0	0	0	0	0	44840	44840	0	0	0	0
CL_2	kg/hr	0	41	0	41	0	0	41	41	0	0	0	0
NH_3	kg/hr	0	0	0	0	0	0	37	37	0	0	0	0
H_2S	kg/hr	0	0	0	0	0	0	50	50	0	0	0	0
C_2H_6	kg/hr	0	0	0	0	0	0	31	31	0	0	0	0
C_2H_4	kg/hr	0	0	0	0	0	0	425	425	0	0	0	0
TAR ($C_{10}H_8$)	kg/hr	0	0	0	0	0	0	1	1	0	0	0	0
C_2H_2	kg/hr	0	0	0	0	0	0	370	370	0	0	0	0

Table A. 19 - Mass and Energy Balance: Steam and Power generation (cont)

	Units	**STEAM90.TOT**	**STEAM20.TOT**	**STEAM4.AGR**	**STEAM.MILL**	**STEAM.GAS**	**STEAM.REF**	**STEAM.LOCAT**	**COND**
Temperature	C	520	330	168.7896821	235	310	310	235	47.9
Pressure	bar	90	20	4	2.5	2.5	2.533125	2.5	0.11
Enthalpy Flow	MW	-1017	-169	-46	-962	-147	-77	-1	-1
Mass Flows	kg/hr	294263	47320	12461	265913	41129	21475	289	316
H2O	kg/hr	294262.7387	47319.95337	12460.53747	265913.3791	41129.49266	21475.34666	288.5119046	316

*during season

Table A. 20 - Mass and Energy Balance: Steam and Power generation (cont)

	Units	**STEAM90.TOT**	**STEAM20.TOT**	**STEAM4.AGR**	**STEAM.MILL**	**STEAM.GAS**	**STEAM.REF**	**STEAM.LOCAT**	**COND**
Temperature	C	520	330	168.7896821	-	310	310	235	47.7
Pressure	bar	90	20	4	-	2.5	2.533125	2.5	0.11
Enthalpy Flow	MW	-1017	-169	-46	-	-147	-77	-1	-1008
Mass Flows	kg/hr	294263	47320	12461	-	41129	21475	289	266228
H2O	kg/hr	294263	47320	12461	-	41129	21475	289	266228

*during off-season

iii. - Economic estimations

The main economic parameters necessary for the analysis are the investment costs and operational costs. With this in mind, Table A. 21 presents the considered investment costs for the equipment, while Table A. 22 presents the costs for the different inputs. For the fixed investment costs and inputs costs of the sugarcane mill, these values were obtained from the VSB framework [1].

Table A. 21 - Equipment purchase and installed costs

	Capacity (base)		Equipment cost		Year	Ref	Installed Cost (base)		Scalled capacity		Scale factor	Local. Factor	Equipment cost		Installed Cost (base)	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
1G ethanol plant	-	-	-		-	VSB [1]	-		4	M ton sugarcane/year	-	-			107.49	M US$
LCM preprocessing																
straw reception and processing	-	-	-		-	VSB [1]	-		349703.77	ton straw/year	-	-			9.53	M US$
Dryer	74	ton evaporated water/h	7.63	M US$	2002	[12]	18.85	M US$	73.68	ton evaporated water/h	1	1.325	15.45	M US$	38.17	M US$
Syngas production																
Gasification + Tar reformer	68.55	ton biomass (d.b)/h	19.8	M US$	2010	[6]	45.74	M US$	102.82	ton biomass (d.b)/h	1	1.325	48.75	M US$	112.61	M US$
heat integration*						[6]									4.03	M US$
compression	28.934	MW (energy consumption)	16.81	M US$	2005	[9]	41.521	M US$	24.14	MW (energy consumption)	0.62	1.325	25.82	M US$	63.78	M US$
AGR	66.38	ton acid gas/h	6.79	M US$	2007	[2]	20.37	M US$	57.49	ton acid gas/h	0.75	1.325	9.34	M US$	28.02	M US$
Sulfur recovery	0.042	ton sulfur/h	2.92	M US$	2002	[6]	3.942	M US$	0.04	ton sulfur/h	0.75	1.325	4.68	M US$	6.31	M US$
Fuel synthesis																
FT reactor	100	MW (FT liquids)			2000	[10]	16.7	M US$	100	MW (FT liquids)	1	1.325			28.77	M US$
other	113.7	ton syngas/h	4.51	M US$	2007	[2]	4.51	M US$	71.2	ton syngas/h	1	1.325	0.8	M US$	0.8	M US$
Hydroprocessing	0.159	m^3 liquid fuels/day	0.004	M US$	2007	[13]	0.009	M US$	238.36	m^3 liquid fuels/day	1	1.325	9.19	M US$	21.22	M US$
Storage	1000	m^3 liquid fuels/month	0.3147	M US$	2014		0.727	M US$	4716.66	m^3 liquid fuels/month	1	1.325	2.088	M US$	4.823	M US$

	Capacity (base)		Equipment cost		Year	Ref	Installed Cost (base)		Scalled capacity		Scale factor	Local. Factor	Equipment cost		Installed Cost (base)	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Steam system and power generation																
Water treatment	216.3	ton/h	2.47	M US$	2007	[6]	2.841	M US$	347	ton/h	0.7	1.325	5.27	M US$	6.06	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[6]	1.597	M US$	347	ton/h	0.3	1.325	1.17	M US$	2.831	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.29	M US$	2007	[6]	0.702	M US$	347	ton/h	0.65	1.325	0.49	M US$	1.186	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	31.9	MW	0.7	1	4.18	M US$	7.52	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	65.94	MW	0.7	1	13.5	M US$	24.26	M US$
Gas turbine	-	-	-	-	-	-	-	-	71.13	MW	-	-	-	-	35.61	M US$
Transmission/stations	-	-	-	-	-	-	-	-	141.74	MW	-	-	-	-	19.65	M US$
Heat integration	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.88	M US$
Utilities																
Air systems	119	ton biomass/h	0.3	M US$	2007	[6]	0.57	M US$	187.93	ton biomass/h	0.3	1.325	0.53	M US$	1	M US$
Cooling water systems	2660	ton water/h	0.66	M US$	2007	[6]	1.478	M US$	5681.91298	ton water/h	0.6	1.325	1.59	M US$	3.57	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[6]	1.909	M US$	303.79	ton flue gas/h	0.65	1.325	1.02	M US$	2.35	M US$
Purge water treatment	0.1	ton water/h	0.36	M US$	2007	[6]	0.9	M US$	0.21	ton water/h	0.65	1.325	0.89	M US$	2.22	M US$
Chemicals storage	119	ton biomass/h	0.5	M US$	2007	[6]	0.98	M US$	187.93	ton biomass/h	0.65	1.325	1.03	M US$	2.02	M US$

Table A. 22 - Inputs costs (Biomass-to-liquids process)

Variable Operating Costs	**Reference cost**		**Ref.**	**Year**	**Value**		**Total cost**	
Mill chemicals inputs	-	-	VSB [1]	2019	-	-	1.25	M US$/year
Other mill inputs cost	-	-	VSB [1]	2019	-	-	1.03	M US$/year
LO-CAT Chemicals	176	US$/ton of S produced	[2]	2007	351.8	ton of S/year	0.09	M US$/year
DEA make-up	2.06	US$/kg	[14]	2019	96286.9	kg amine/year	0.2	M US$/year
Hydroprocessing	11.35	$/m3 produced	[13]	2007	78659.1	m3/year	1.33	M US$/year
FT Catalyst (Cobalt)	33.07	US$/kg	[2]	2007	100.9	ton/year	4.96	M US$/year
Tar reformer catalyst	65.48	US$/kg	[6]	2007	0.0041	ton/h	1.91	M US$/year
Olivine	172.9	US$/ton	[6]	2004	21987.8	kg/year	8.36	M US$/year
ZnO Guard Bed	12536.64	US$/m3	[9]	2005	12.3	m^3/year	0.3	M US$/year
PSA Packing	65180.33	US$/hourly ton syngas in/year	[2]	2007	0.7	ton/h	0.07	M US$/year
Chemicals for water System	0.03	US$/m3	VSB [1]	2017	1318892.9	m3/year	0.04	M US$/year
Steam system	0.03	US$/ton steam	VSB [1]	2017	2705336.4	ton/h	0.09	M US$/year

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Annex B - Supplementary Material (Chapter V)

Supplementary material

i. - First generation ethanol production

Table B. 1 - Main parameters adopted in the agricultural simulations

Agricultural parameters	Value	Unit	Source
Sugarcane yield	80	TC/ha	(WATANABE et al., 2020)
Straw recovery	2.4	t_{db}/ha	Assumed
Straw recovery fraction	50	%	Assumed
Straw recovery method	bales	-	Assumed
Mean transportation distance (mean radius – r)	36	km	Calculated

db: dry basis; ha: hectare; TC = tonnes of cane

*costs calculated for a mill processing 5 million tons of sugarcane per year.

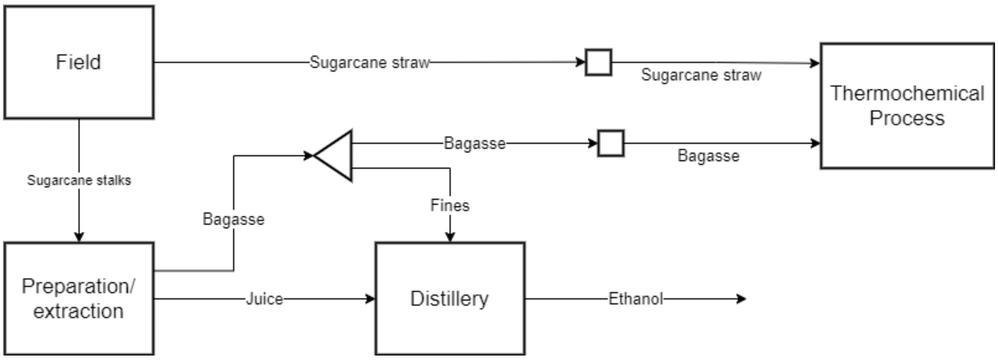

Figure B. 1 - Simplified flowchart for the 1G mill

Table B. 2 - Main parameters for the industrial stage of the 1G sugarcane mill

Industrial Parameters	Value	Unit	Reference
Overall process			
Total sugarcane processed	4	Million TC	Assumed
Operational days	200	Days/year (season)	
	330	Days/year (season + off season)	
Reception and cleaning			
Electricity demand (conveyors and fans)	0.692	kWh/t	[1]
Extraction			
Efficiency of sugar extraction in the mills	96	%	
Amount of imbibition water	280	kg/TC	
Bagasse moisture	50	%	
Fermentation/distillation			
Fermentation efficiency	90	%	
Wine ethanol concentration	80	g/l	

For the fixed investment costs and inputs costs of the sugarcane mill, these values were obtained from the VSB framework [1].

ii. - Simulation description

The process of simulation and evaluation of the proposed route used the Virtual Sugarcane Biorefinery – VSB [1]. The VSB is a tool that integrates different computational platforms such as Aspen Plus®, SimaPro®, and electronic spreadsheets for the technical, economic, environmental, and social analyses. This tool allows the decision-making process by considering the agricultural technology, passing through the industrial processes, and reaching up to the logistics of use and distribution of the biofuel. This platform, developed by LNBR, is mainly utilized to evaluate the sugarcane sector but can also be adapted to assess different biomasses and industrial processes. This platform already contains a detailed representation of the sugar mill industrial process including all the agricultural stage for sugarcane harvesting.

This database, however, does not contain the thermochemical processes of pyrolysis and gasification. The explanation of the simulation of these processes are as follow.

ii.i. - Bio oil production

(1) Preprocessing

The straw (baled) is chopped and sieved and is dried together with the bagasse to 10 wt.% moisture. Initially, the straw contains approximately 20-30% moisture, while for the bagasse this content is around 50%. The main consumption of this step is the electricity consumed on the sieves and chopper (total of 3.73 kWh/ton$_{\text{straw d.b.}}$) and the heat demand on the dryer (1.5 MJ/kg$_{\text{evaporated water}}$).

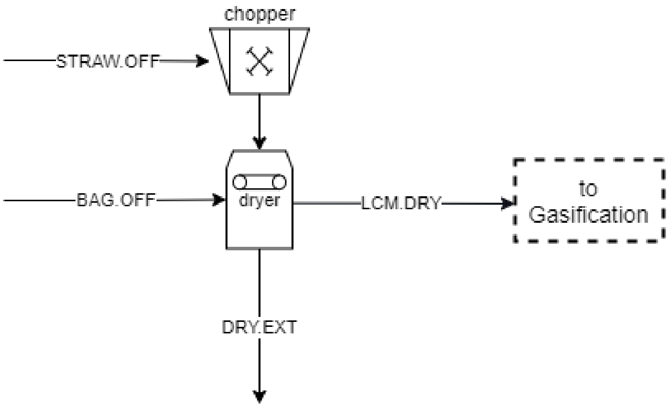

Figure B. 2 - Flowchart of the preprocessing of the lignocellulosic material

(2) Fast pyrolysis

The simulation of the fast pyrolysis process considered a kinetic approach as proposed by Ranzi et al. [2]. This approach considers the decomposition of cellulose, hemicellulosis, lignin and extractives into intermediate components. These components are further converted into levoglucosan, C5-C6 chemicals and pyrolytic products. For these reaction, we considered that:

i) Cellulose (CEL) is converted to its intermediate compost CELLA
ii) Hemicellulose generates two intermediate components (HCE1 and HCE2)
iii) Lignin is represented by three components: LIGC – rich in carbon; LIGH – rich in hydrogen; and LIGO – rich in oxygen

iv) Lignin originates LIGCC and LIGOH

v) The extractives are represented by tanins (TAN) and triglycerides (TGL)

The chemical structure for each component is available on Ranzi et al. [2], and Table B. 3 presents the reactions. The simulation of the process was performed using the software Aspen Plus (v 9.0) and by adapting the work from Salina et al. [3]. Table B. 4 presents the main components for the simulation.

Table B. 3 - Main reactions for the pyrolysis process

Reaction	**A (s^{-1})**	**Ea (kcal/mol)**
Cellulose		
CELL → CELLA	$1,5.10^{14}$	47
CELLA → 0,4 HAA + 0,05 GLYOX + 0,15 CH3CHO + 0,25 HMFU + 0,35 ALD3 + 0,15 CH3OH + 0,3 CH2O + 0,61 CO + 0,36 CO2 + 0,05 H2 + 0,93 H2O + 0,02 HCOOH + 0,05 C3H6O2 + 0,05 CH4-T + 0,2 H2-T + 0,61 CHAR	$2,5.10^{6}$	19,1
CELLA → LVG	3,3.T	10
CELL → 5 H20 + 6 CHAR	$6,0.10^{7}$	31
Hemicellulose		
HCE → 0,70 HCE1 + 0,30 HCE2	$1,0.10^{10}$	31
HCE1 → 0,6 XYLAN + 0,2 C3H6O2 + 0,12 GLYOX + 0,2 FURF + 0,4 H2O + 0,08 H2-T + 0,16 CO	3,0.T	11
HCE1 → 0,4 H2O + 0,79 CO2 + 0,05 HCOOH + 0,69 CO + 0,01 CO-T + 0,01 CO2-T + 0,35 H2-T + 0,3 CH2O + 0,9 COH2-T + 0,625 CH4-T + 0,375 C2H4-T + 0,875 CHAR	$1,8.10^{-3}$.T	3
HCE2 → 0,2 H2O + 0,275 CO + 0,275 CO2 + 0,4 CH2O + 0,1 C2H5OH + 0,05 HAA + 0,35ACAC + 0,025 HCOOH + 0,25 CH4-T + 0,3 CH3OH-T + 0,225 C2H4-T + 0,3 CO2-T + 0,725 COH2-T + CHAR	$5,0.10^{9}$	31,5
Lignin		

LIGC → 0,35 LIGCC + 0,1 COUMARYL + 0,08 PHENOL + 0,41 C2H4 + 1,0H2O + 0,7 COH2-T + 0,3 CH2O + 0,32 CO + 0,495 CH4-T + 5,735 CHAR	1,0.10^{11}	37,2
LIGH → LIGOH + 0,5 ALD3 + 0,5 C2H4 + 0,2 HAA + 0,1 CO + 0,1 H2-T	6,7.10^{12}	37,5
LIGO → LIGOH + CO2	3,3.10^{8}	25,5
LIGCC → 0,3 COUMARYL + 0,2 PHENOL + 0,35 HAA + 0,7 H2O + 0,65 CH4 + 0,6 C2H4 + H2 + 1,4 CO + 0,4 CO-T + 6,75 CHAR	1,0.10^{4}	24,8
LIGOH → 0,9 LIG + H2O + 0,1 CH4 + 0,6 CH3OH + 0,05 H2-T + 0,3 CH3OH-T + 0,05 CO2 + 0,65 CO + 0,6 CO-T + 0,05 HCOOH + 0,85 COH2-T + 0,35 CH4-T + 0,2 C2H4-T + 4,25 CHAR + 0,025 HMWL + 0,1 ACROL	1,0.10^{8}	30
LIG → 0,7 FE2MACR + 0,3 ANISOLE + 0,3 CO + 0,3 G{CO} + 0,3 CH3CHO	4,0.T	12
LIG → 0,6 H2O + 0,4 CO + 0,2 CH4 + 0,4 CH2O + 0,2 G{CO} + 0,4 G{CH4} + 0,5 C2H4-T + 0,4 CH3OH-T + 2 COH2-T + 6 CHAR	8,3.10^{-2}.T	8
LIG → 0,6 H2O + 2,6 CO + 1,1 CH4 + 0,4 CH2O + C2H4 + 0,4 CH3OH + 4,5 CHAR	1,0.10^{7}	24,3
Extractives		
TANN → 0,85 FENOL + 0,15 PHENOL-T + CO-T + H2O + ITANN	20	10
ITAN → 5 CHAR + 2 CO + H2O + COH2-T	1,0.10^{3}	25
TGL → ACROL + 3 FFA	7,0. 10^{12}	45,7
Components trapped on the char		
CO2-T → CO2	1,0 10^{6}	24
CO-T → CO	5,0 10^{12}	50
COH2-T → CO+H2	1,5 10^{12}	71
H2-T → H2	5,0 10^{11}	75
CH4-T → CH4	5,0 10^{12}	71,5

CH3OH-T → CH3OH	$2,0\ 10^{12}$	50
C2H4-T → C2H4	$5,0\ 10^{12}$	71,5
PHENOL-T → PHENOL	$1,5\ 10^{12}$	71
Water evaporation		
ACQUA → H2O	1,0 T	8

Table B. 4 - Components for the simulation of fast pyrolysis

ID do componente	**Tipo**	**Nome do componente**	**Alias**
ACAC	Conventional	ACETIC-ACID	C2H4O2-1
ACROL	Conventional	ACROLEIN	C3H4O
ALD3	Conventional	N-PROPIONALDEHYDE	C3H6O-3
ANISOLE	Conventional	METHYL-PHENYL-ETHER	C7H8O-1
BIOMASS	Nonconventional		
C2H4	Conventional	ETHYLENE	C2H4
C2H4-T	Conventional	ETHYLENE	C2H4
C2H5OH	Conventional	ETHANOL	C2H6O-2
C3H6O2	Conventional	ACETOL	C3H6O2-D1
CEL	Solid	LEVOGLUCOSAN	C6H10O5-N1
CELLA	Solid	LEVOGLUCOSAN	C6H10O5-N1
CH2O	Conventional	FORMALDEHYDE	CH2O
CH3CHO	Conventional	ACETALDEHYDE	C2H4O-1
CH3OH	Conventional	METHANOL	CH4O
CH3OH-T	Conventional	METHANOL	CH4O
CH4	Conventional	METHANE	CH4
CH4-T	Conventional	METHANE	CH4
CHAR	Solid	CARBON-GRAPHITE	C

ASH	Nonconventional		
CO	Conventional	CARBON-MONOXIDE	CO
CO2	Conventional	CARBON-DIOXIDE	CO2
CO2-T	Conventional	CARBON-DIOXIDE	CO2
CH2O-T	Conventional	FORMALDEHYDE	CH2O
CO-T	Conventional	CARBON-MONOXIDE	CO
COUMARYL	Conventional	ETHYL-BENZOATE	C9H10O2
FE2MACR	Conventional	TRANS-2,5-DIMETHOXYCINNAMIC-ACID	C11H12O4-N2
FFA	Conventional	LINOLEIC-ACID	C18H32O2
FURF	Conventional	FURFURAL	C5H4O2
GLYOX	Conventional	GLYOXAL	C2H2O2
H2	Conventional	HYDROGEN	H2
H2-T	Conventional	HYDROGEN	H2
H2O	Conventional	WATER	H2O
HAA	Conventional	GLYCOL-ALDEHYDE	C2H4O2-D1
HCE1	Solid	GLUTARIC-ACID	C5H8O4
HCE2	Solid	GLUTARIC-ACID	C5H8O4
HCEL	Solid	GLUTARIC-ACID	C5H8O4
HCOOH	Conventional	FORMIC-ACID	CH2O2
HFMU	Conventional	5-HYDROXYMETHYLFURFURAL	C6H6O3-N5
HMWL	Conventional		
ITANN	Conventional		
LIG	Solid	TRANS-3,4-DIMETHOXYCINNAMIC-ACID	C11H12O4
LIGC	Solid		
LIGCC	Solid		
LIGH	Solid		

LIGO	Solid		
LIGOH	Solid		
LVG	Conventional	LEVOGLUCOSAN	C6H10O5-N1
N2	Conventional	NITROGEN	N2
NO	Conventional	NITRIC-OXIDE	NO
NO2	Conventional	NITROGEN-DIOXIDE	NO2
O2	Conventional	OXYGEN	O2
PHENOL	Conventional	PHENOL	C6H6O
PHENOL-T	Conventional	PHENOL	C6H6O
TANN	Solid	CATECHIN-HYDRATE	C15H12O7
TGL	Solid		
WATER	Conventional	WATER	H2O
XYLAN	Conventional	GLUTARIC-ACID	C5H8O4
CL	Conventional	CHLORINE	CL2
S	Conventional	SULFUR	S
CL2	Conventional	CHLORINE	CL2
H2S	Conventional	HYDROGEN-SULFIDE	H2S
HCN	Conventional	HYDROGEN-CYANIDE	CHN
N2-BIOM	Conventional	NITROGEN	N2

The process simulation follows three main hierarchies: the fast pyrolysis, the recovery of products, and the combustion and energy generation.

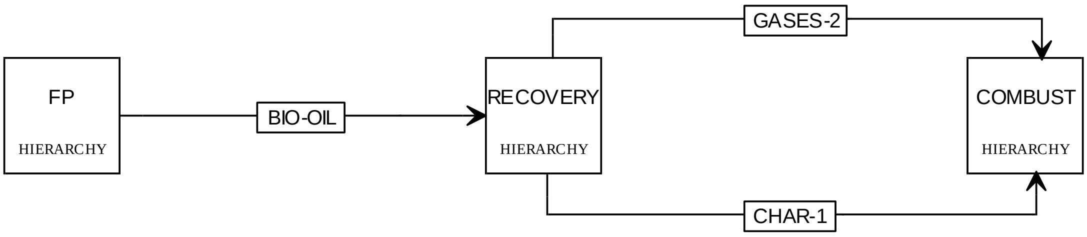

Figure B. 3 - Overall process for bio-oil production

On the FP hierarchy, the non-conventional stream of biomass is converted to the components CEL, HCEL, LIGH, LIGC, LIGO, TGL and TANN based on proximate and ultimate analysis composition. A RKINETIC block with the reactions from Table B. 3 convert these components. A stream of pressurized and heated nitrogen is added on the reactor. A block (R-IMPUR) considers the formation of impurities (sulfur and nitrogen). The product stream (PROD2) is sent to solid separator (CYCLONE), and the resulting vapor phase is cooled (QUENCH block) with the contact with a reflux of cooled bio-oil. The bio-oil is separated with two condensers (CON1 and CON2) and flashes (SEP1 and SEP2). The gases and char stream is decomposed into its elements (block CHARDEC) and combusted on the CHARCOMB block.

For the standalone configuration (scenario 3), there is no consumption of steam on the process. It is hen considered that the char and gases are combusted on a boiler to generate steam that is totally used for electricity production. This electricity is enough to supply the demand of the process.

For the integrated configuration (scenario 4), the presence of the 1G mill raises the electricity consumption, also adding a demand of steam. To supply this energy demand, the hot gases from the combustion of char and FP gases is used on a combined cycle, first going through a turbine, and then generating steam.

In both standalone and integrated configurations the heat from the condensers are used to generate additional steam.

Table B. 5 presents the inputs and conditions for the main blocks for the FP simulation, while Figure B. 3 and Figure B. 5 present the flowchart of the process with the main streams.

Table B. 5 - Inputs for the FP simulation

Hierarchy	**Block**	**Type**	**Function**	**Op. conditions/*Inputs***
FP	COMPR1	COMPR	N_2 compression	Isentropic compressor, 1.5 bar
FP	PREAQ	HEATER	N2 heating	475 °C
FP	RDEC	RYield	Convert proximate analysis into chemical composition	25 °C, 1 bar,
FP	RKINETIC	RCSTR	FP reactions	480 °C, 1,5 bar, 1 s residence time, vapor phase,
FP	R-IMPUR	RStoic	Impurities formation	480 °C, 1,5 bar, formation reactions of HCN and H_2S (100% conversion)
FP	MIXQ	Mixer	Soma das correntes de valor dos blocos de pirólise	n.a.
RECOVERY	CYCLONE	SEP	Solid separation	*Split ratio* = 0,99 for all biochar components
RECOVERY	QUENCH	MIXER	Bio oil cooling	n.a.
RECOVERY	CON1	HEATER	Condensable cooling and recovery	75 °C,
RECOVERY	SEP1	FLASH	Condensate recovery	Adiabatic,
RECOVERY	CON2	HEATER	cooling	25 °C
RECOVERY	SEP2	FLASH	Condenstate recovery	Adiabatic
RECOVERY	REFLUX	SPLITTER		*Split ratio* = 0,9 (stream REF2)
RECOVERY	RESF	HEATER	Cooling	25 °C
RECOVERY	MIX2	MIXER		n.a.
RECOVERY	PURG	SPLITTER		Split fraction = 0 (stream PG)

COMBUST	CHARDEC	RStoic	Convert non conventional into conventional stream	475 °C
COMBUST	CHARCOMB	RStoic	Biochar combustor	1000 °C
COMBUST	COMPR2	COMPR	Air compressor	Isentropic compressor , 1,5 bar
COMBUST	B7	HEATER	cooling	n.a.
COMBUST	ASHSEP	SEP	Ashes recovery	*Split ratio* = 1,0 (ashes)
COMBUST	B9	HEATER	Flue gas cooling	500 °C

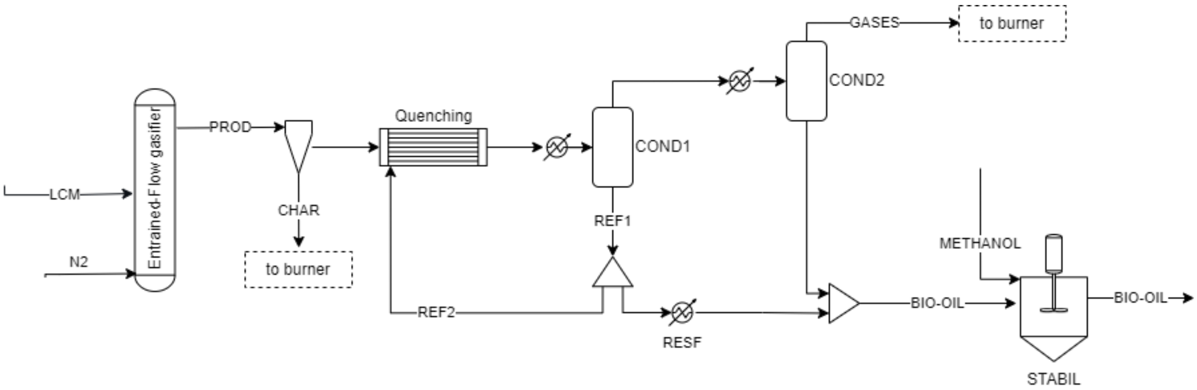

Figure B. 4 - Fast pyrolysis and product recovery

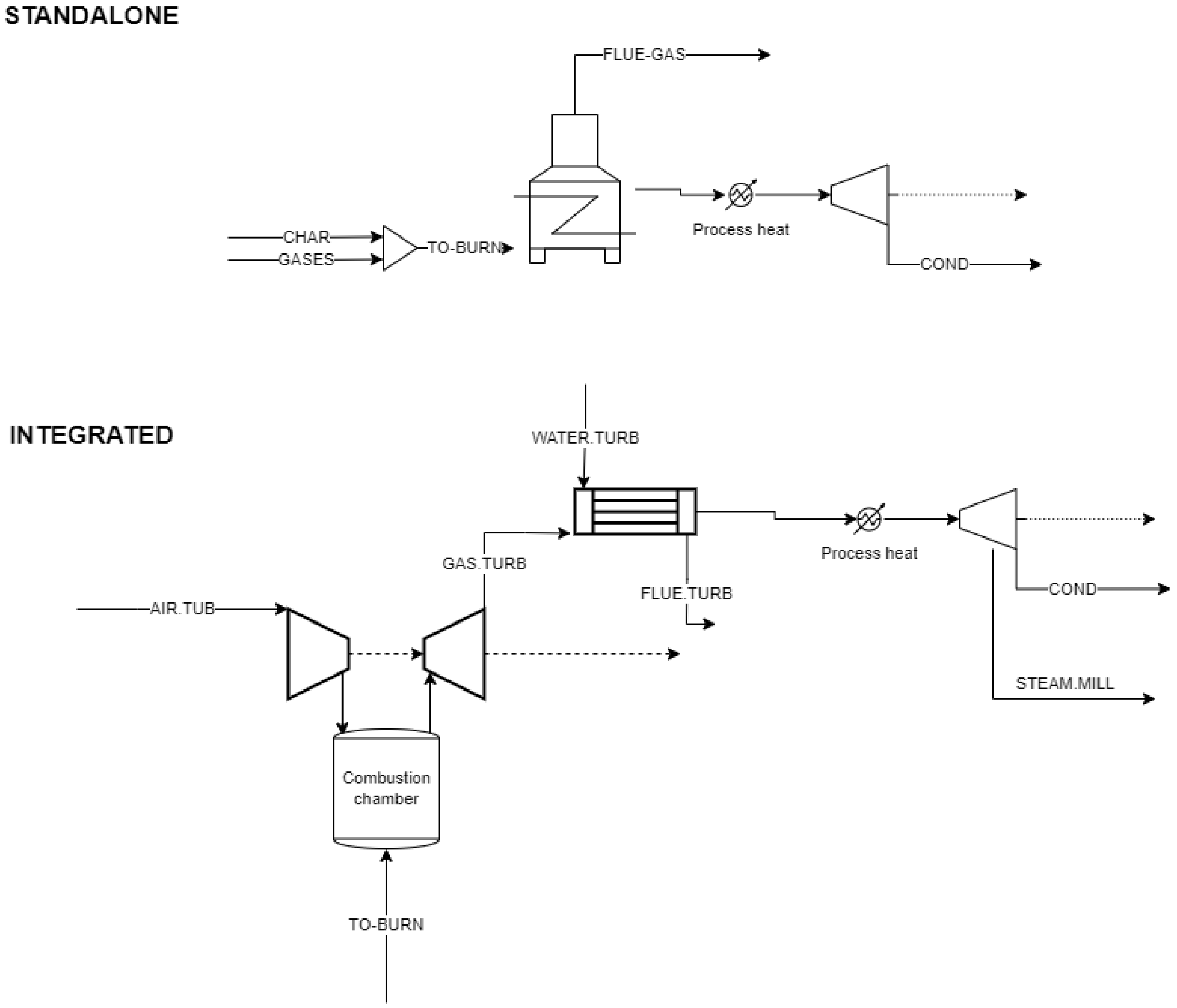

Figure B. 5 - Power/steam generation for the bio-oil production process for a standalone scenario, and a integrated into a 1G mill case

ii.ii. - GFT route - Scenario 1

Table B. 6 presents the proprieties considered for the lignocellulosic materials (bagasse + straw) for the simulation of the GFT process into the Aspen Plus software. The remaining components were obtained from the already existing VSB simulation framework. Table B. 7 present some components that are used to simulate more complex substances, such as the products from the FT synthesis being represented by linear chain hydrocarbons.

Table B. 6 - Characterization of the lignocellulosic material (reference: VSB [1]*)*

	wt. % (d.b)
Proximate analysis	
Fixed carbon	16.79
Volatile matter	80.06
Ash	3.15
Ultimate analysis	
Ash	3.15
Carbon	46.69
Hydrogen	5.72
Nitrogen	0.32
Chlorine	0.04
Sulfur	0.05
Oxygen	44.03

Table B. 7 - Model components for the simulation of more complex components

Component	**Model component**	**Formula**	**Reference**
Minerals	Potassium-oxide	K2O	VSB [1]
Organic acids	Trans-aconitic-acid	C6H6O6	VSB [1]
Salts	Potassium-chloride	KCL	VSB [1]
Soil	Silicon-dioxide	SIO2	VSB [1]
C5	N-pentane	C5H12-1	[4]
C6	N-hexane	C6H14-1	[4]
C7	N-heptane	C7H16-1	[4]
C8	N-octane	C8H18-1	[4]
C9	N-nonane	C9H20-1	[4]
C10	N-decane	C10H22-1	[4]
C11	N-undecane	C11H24	[4]
C12	N-dodecane	C12H26	[4]
C13	N-tridecane	C13H28	[4]
C14	N-tetradecane	C14H30	[4]
C15	N-pentadecane	C15H32	[4]
C16	N-hexadecane	C16H34	[4]
C17	N-heptadecane	C17H36	[4]
C18	N-octadecane	C18H38	[4]
C19	N-nonadecane	C19H40	[4]
C20	N-eicosane	C20H42	[4]
C21	N-heneicosane	C21H44	[4]
C22	N-docosane	C22H46	[4]
C23	N-tricosane	C23H48	[4]
C24	N-tetracosane	C24H50	[4]
C25	N-pentacosane	C25H52	[4]
Waxes	N-triacontane	C30H62	[4]

MDEA	Methyl-diethanolamine	C5H13NO2	[5]
MDEA+	Mdea+	C5H14NO2+	[5]
Tar	Naphthalene	C10H8	[6]

Figure B. 6 presents the overview of the simulation flowchart for scenario 1. Sugarcane stalks are retrieved from the field are destined to the preparation/extraction stage of the mill. The juice is destined to the distillery (where ethanol is produced) and bagasse is sent to the thermochemical process, with some fraction diverted to the distillery. Sugarcane straw left on the field is collected in the form of bales and sent directly to the BtL process. It is important to highlight that only the industrial process is contemplated in this simulation. The mill simulation is already established into the VSB framework and is detailed elsewhere [1]. The results for the mill are presented for the season period (200 days/year) so the streams of bagasse and straw are corrected to consider the whole period (330 days/year). Electricity and steam (2.5 bar) demands were calculated from the VSB framework and are dependent on the mill capacity.

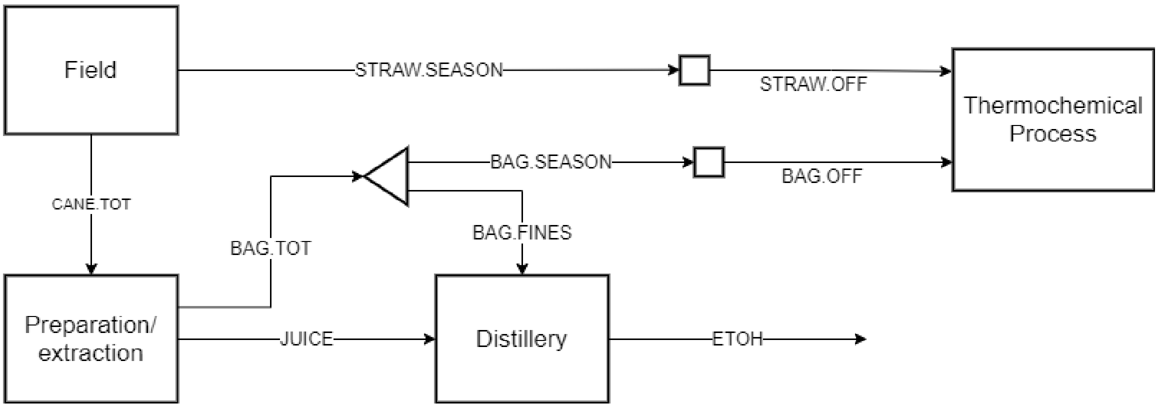

Figure B. 6 - Overall flowchart of the integrated plant

(1) Preprocessing

The first step of the BtL process is the preprocessing of the LCM (Figure B. 7). The baled straw is chopped and sieved, and the resulting stream, together with the bagasse is dried to 10 wt.% moisture. Initially, the straw contains approximately 20-30% moisture, while for the bagasse this content is around 50%. This step consumes 3.73 kWh/ton$_{\text{straw d.b.}}$) of electricity, and 1.5 MJ of heat/kg$_{\text{evaporated water}}$.

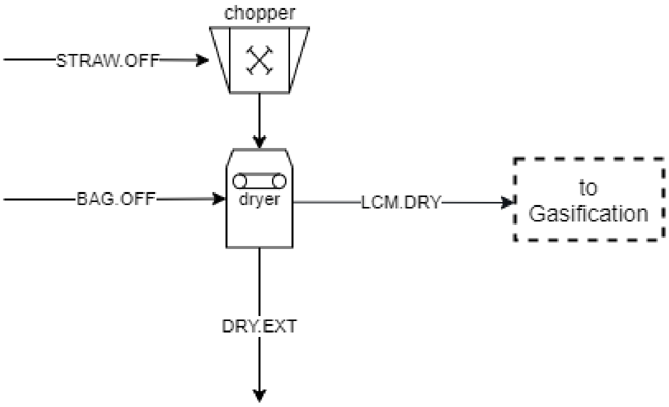

Figure B. 7 - Flowchart of the preprocessing of the lignocellulosic material

(2) Gasification

Figure B. 8 presents the simplified flowchart of the gasification step. It was considered a low-pressure indirectly-heated circulating fluidized bed gasifier operating with steam (2.5 bar) at a ratio of 0.4 ton of steam per ton of dry biomass. The gasification simulation considered the correlations obtained by Bain et al [7] from the Battelle Columbus Laboratory (BCL). These correlations assume the form from Eq. 01 dependent on the temperature (°F). Table B. 8 shows the values for each parameter. The temperature considered in the simulation was the equilibrium temperature obtained by Dutta et al. [8] (gasifier at 870 °C and combustor at 980 °C):

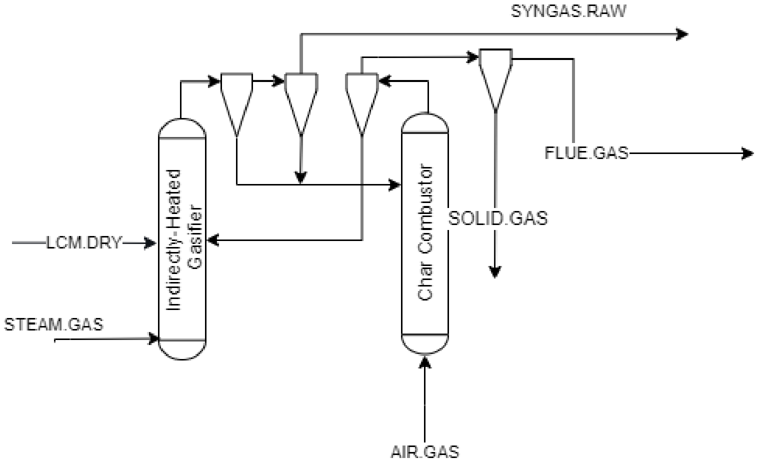

Figure B. 8 - Flowchart of the gasification process

$$Y = a + b.T + c.T^2$$ Eq. B.01

Table B. 8 - Correlation parameters for gasification yields calculations [7]

Variable (Y)	**a**	**b**	**c**	**Units**[b]
Dry syngas (mass)	0.1555	-0.0002206	0.000000376	lb/lb dry biomass
CO	133.4600	-0.1029	0.000028792	mole % dry gas
CO_2	-9.5251	0.037889	-0.000014927	mole % dry gas
CH_4	-13.8200	0.044179	-0.000016167	mole % dry gas
C_2H_4	-38.2580	0.058435	-0.000019868	mole % dry gas
C_2H_6	11.1140	-0.011667	0.000003064	mole % dry gas
H_2	17.9960	-0.026448	0.00001893	mole % dry gas
C_2H_2	-4.3114	0.0054499	-0.000001561	mole % dry gas
Tar ($C_{10}H_8$)	0.045494	-0.000019759	-	lb/lb dry biomass
Water conversion	0.2896	-0.00089048	0.00000043384	%

The produced amount of syngas as well as the quantities of each component are calculated from these correlations. This allows us to estimate the flow of each component on the resulting syngas. With the total flow of carbon present on the biomass and the carbon present in the syngas, the residual carbon is attached to the char. The same reasoning allows us to calculate the oxygen atomic content on the char.

8.3% of the sulfur and 6.6% of the nitrogen present on the biomass are transferred to the char [8]. The remaining atoms of these components are present in the form of H_2S and NH_3 in the syngas. All the chlorine is assumed to be set as HCl in syngas. Through mass balance, the content of hydrogen on the char is calculated. All ash is considered to be part of char. Further elaboration of the calculations can be found on Bressanin et al [9].

99.99% of the solid in the syngas are separated and sent to the combustor. 99% of the olivine from the combustor is separated from flue gas and recycled to the gasifier. Fresh olivine is added at a rate of 27 kg/kg of dry biomass [8]. The flue gas from the combustor is sent to heat integration to generate steam.

(3) Syngas cleaning

The first step of the cleanup process (Figure B. 9) is the reforming, where methane, tars, and other light hydrocarbons are converted to CO and H_2, and NH_3 becomes N_2 and H_2. Table

B. 9 presents the reactions considered for this stage, and the respective conversions considered [4,8,10]. Besides these reactions, it was also considered that the reactor also promotes Water-gas-shift reaction (Eq. B.02). Steam is added to the reactor to shift this equilibrium and correct the H_2/CO molar ratio to 2.1 at the entrance of the FT reactor.

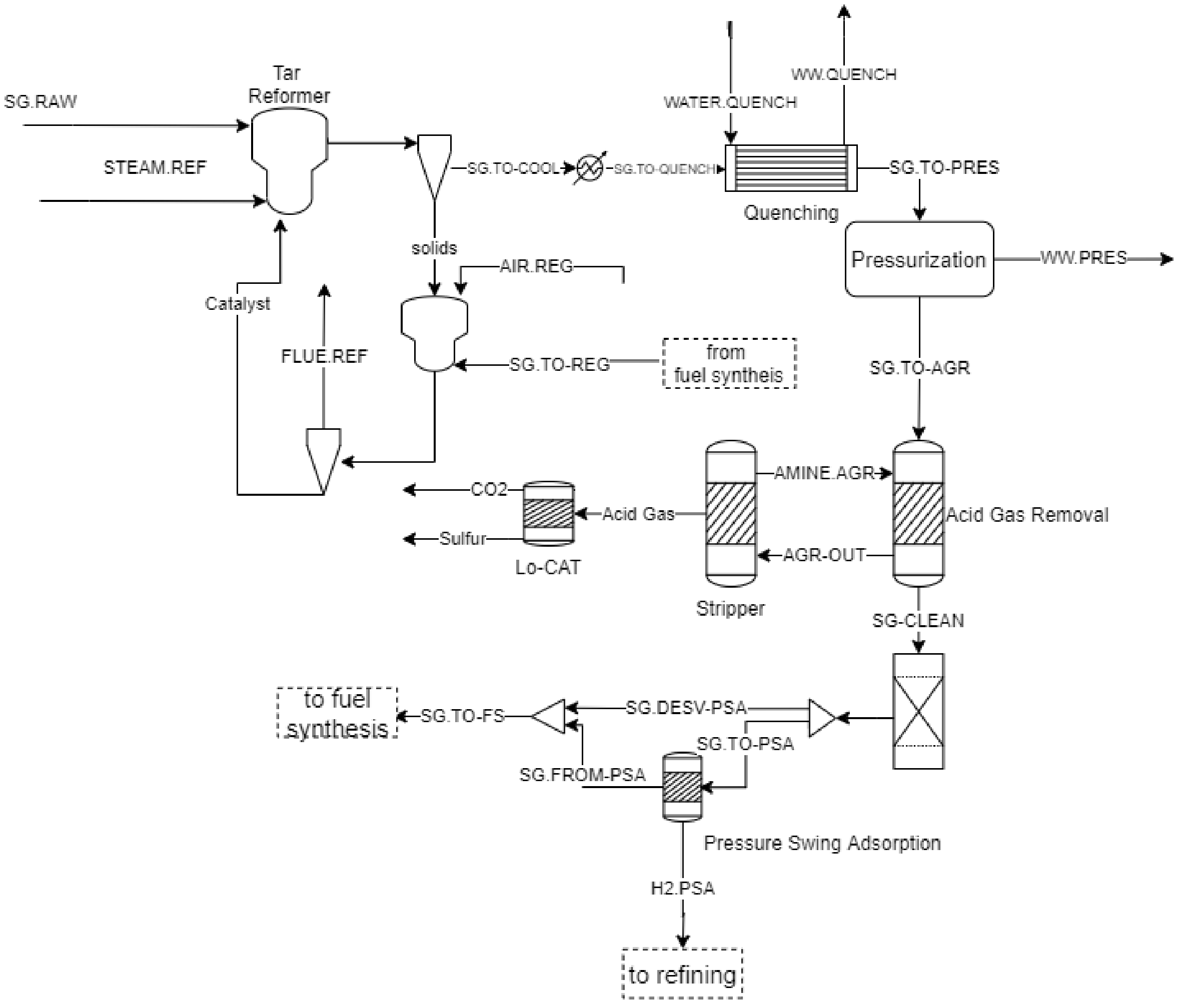

Figure B. 9 - Flowchart for the syngas cleanup processes (LCM GFT)

Table B. 9 - Reactions and conversions for the reforming process

Reaction	Conversion	Component

TAR + 10 H_2O → 10 CO + 14 H_2	0.99	TAR ($C_{10}H_8$)
CH_4 + H_2O → CO + 3 H_2	0.8	CH_4
C_2H_4 + 2 H_2O → 2 CO + 4 H_2	0.9	C_2H_4
2 NH_3 → N_2+ 3 H_2	0.9	NH_3
C_2H_6 + 2 H2O → 2 CO+ 5 H_2	0.9	C_2H_6

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad \text{Eq. B.02}$$

The reforming section also counts with a catalyst regenerator that combusts the deposits from the catalyst particles. This regenerates the activity and supplies heat to the reforming reactions. Air is fed with 20% excess to the regenerator, and some unconverted syngas from the fuel synthesis stage is also supplied to help meet the heat demand. A two-stage cyclone separates the catalyst, and the combustion flue gases are used in heat integration. Around 0.03 kg of catalyst per ton of gas fed to the reformer is considered as make-up to replace the cyclones losses [9].

After reforming the syngas are cooled and sent to a scrubbing system. The first heat exchanger cools the syngas to around 60°C, and the heat is utilized to heat integration and steam generation. The scrubbing system works with a flow rate of 1 liter of water per m^3 of gas. Around 5 kg of fresh makeup, water per ton of circulating water is required [8] and the electricity requirement of this process is assumed to be 0.1 kWh per ton of syngas [11].

The pressurization of the syngas occurs on a 5-stage centrifugal compressor with knock-out drums up to around 25 bar. The calculated energy consumption is around 0.19 kWh/m^3 of syngas.

In this study, it is considered the use of a 30 %wt. methyl diethanolamine solution for the Acid-Gas-Removal (AGR) process. The process was simulated by considering the reactions between the amine and H_2S/CO_2. Table B. 10 shows the considered reactions and the conversion for each component [5,11]. It was considered that 0.01% of the circulating amine is lost and must be made up for. Make-up water is assumed to be enough to maintain the concentration of amine. A flash separator and a stripper column regenerate the amine removing the acid gas, and the lean amine is cooled and cycled back to the absorber. This process consumes 4 bar steam (at a rate of around 3620 MJ per ton of acid gas), around 1.06 kWh of electricity per mass of circulating solvent, and 32.2 tons of cooling water supplied per ton of syngas inlet [11]. A LO-CAT® unit removes the sulfur from the acid gas, and it is assumed that 0.08 t LO-CAT chemical is necessary per ton of sulfur, together with 4.7% of makeup water in sour gas, 0.28 kg of steam per kmol of acid gas, and electricity consumption of 0.5 kWh electricity per kmol of acid gas [11].

Table B. 10 - Reactions and conversions for the acid gas removal process

Reaction	Conversion	Component
MDEA + $H_2S \rightarrow MDEA^+ + HS^-$	0.99	H2S
MDEA + CO_2 + $H_2O \rightarrow MDEA^+ + HCO_3^-$	0.9	CO2

A ZnO bed is used to remove even more sulfur from the syngas to contents below 50 ppb [11]. This process was not directly simulated, but the consumption of fresh catalysts was considered for the analysis. The ZnO is replaced in a period of 1 year, requiring a volume of 48.5 m^3 of catalyst per kg of H_2S remaining on the syngas [11].

A PSA unit deviates part of the hydrogen present on the syngas. This hydrogen is necessary for the hydroprocessing process on the fuel synthesis step. An efficiency of 85% of the removal of hydrogen is assumed, producing a pure H_2 stream [4].

(4) Fuel synthesis

FT synthesis (Figure B. 10) was conducted on a tubular fixed bed reactor, with cobalt catalyst and inlet pressure and temperature of 25 bar and 200 °C. This process produces several hydrocarbons with variable chain lengths, and these products can be described by the Anderson-Schulz-Flory (ASF) distribution. The yield of each hydrocarbon (X_n – Eq 03) is determined by the chain growth probability (α) model, and dependent on the length of the chain (n – number of carbons) [12], as seen on Eq. 04. The calculation of the flow of each hydrocarbon chain (C1 until C25+) follows the detailed steps described by Swanson et al [4]

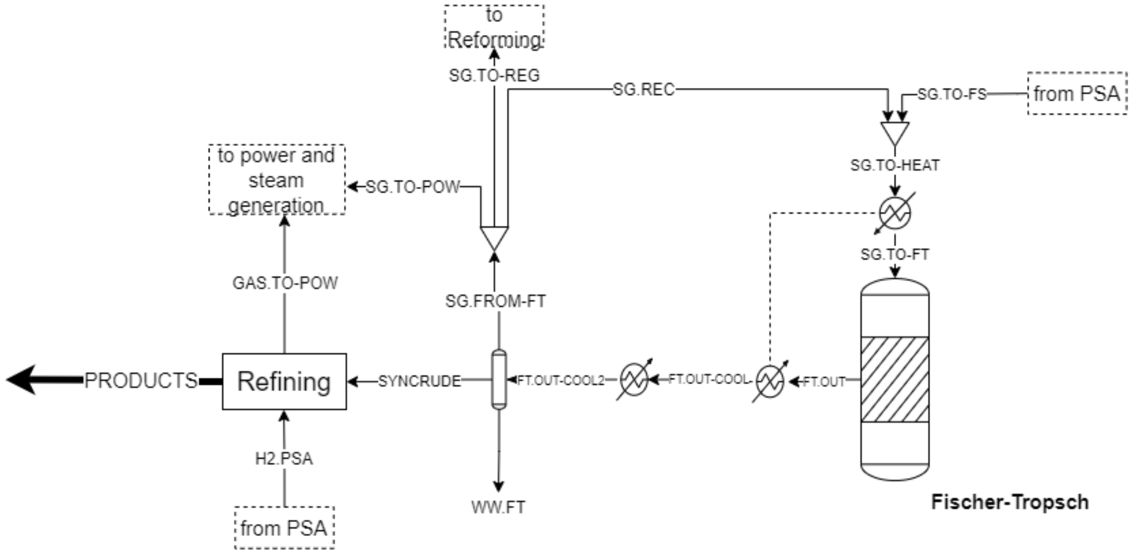

Figure B. 10 - Flowchart for the fuel synthesis processes (LCM GFT)

$$\alpha = \left(\frac{0.2332\, y_{CO}}{y_{CO} + y_{H_2}} + 0.6330\right).[1 - 0.0039(T - 533)] \qquad \text{Eq. B.03}$$

$$X_n = \alpha^{(n-1)}.(1 - \alpha) \qquad \text{Eq. B.04}$$

With y_{co} and y_{H2} the molar fraction of CO and H_2, respectively, and T the temperature (K)

The FT reactions are highly exothermic, and the heat produced on the reactor is utilized to generate steam for the power generation of the plant.

Part of the unconverted syngas is sent to power generation and the regenerator (tar reforming), while the rest is recycled back to the reactor. A per-pass carbon monoxide conversion of 40% [4] is considered.

The liquid products from the FT synthesis are separated into a water stream, and an organic liquid stream, composed of the different hydrocarbons. For the simulation this process of separation was simplified, consisting of a one-stage separator block. For actual applications, during an industrial process, this step would involve at least a two-stage separation to avoid problems such as blockage by wax formation. However, the process can be adequately represented by the current simplification.

The hydrocarbon stream is sent to the refining/hydroprocessing section. The simulation of this stage was done considering the yields proposed by Klerk [13] for a refinery design of a Low-Temperature-Fischer-Tropsch process maximizing the production of kerosene (jetfuel) with co-production of green gasoline. The gases produced are added to the unreacted syngas from the FT reactor destined for energy generation. The composition of the resulting products is shown in Table B. 11. The electricity demand of this process is 0.125 MW/t FT liquids per hour [4], and around 0.43 MWh of energy per ton of FT liquids processed is released to cooling water.

Table B. 11 - Product yields for the hydroprocessing unit [13]

Product	**Mass composition %**
Gasoline	19.6
Jet fuel	57.0
Combustible gases (C_2H_6)	7.4
LPG (C_3H_8)	11.4
Others	4.6

(5) Power and steam generation

The heat integration and power generation of the plant consider the following (Figure B. 11 and Figure B. 12):

- Part of the unconverted syngas/gaseous products are destined to supply heat to the tar reforming catalyst regenerator;
- Deviation of part of the unconverted syngas and the gaseous products to a gas turbine. Excess air is calculated to achieve a temperature of around 610 °C at the inlet of the turbine. This turbine operates with an inlet pressure of 20 bar, with a pressure ratio of 0.05;
- The exhaust from the gas turbine is used to produce superheated steam (90 bar, 520 °C).
- Additional superheated steam (90 bar, 520 °C) from the heat from the cooling of the syngas (before quenching) and the heat of the flue gas from the regenerator (tar reforming) and combustor (gasification);
- 20 bar steam produced from the heat removed from the FT reactor;

- A back-pressure steam turbine with an inlet pressure of 90 bar drops the pressure initially to 20 bar. This outlet is added to the steam produced from the heat integration of the FT reactor and directed to a condensing extraction turbine. Some amount of 4 bar steam is extracted to supply the AGR demands, and 2.5 bar is extracted to meet the demands from the mill, gasification, reforming, and LOCAT processes.
- Electricity produced from these turbines (gas and steam turbines) supplies all the power demand of the plant.

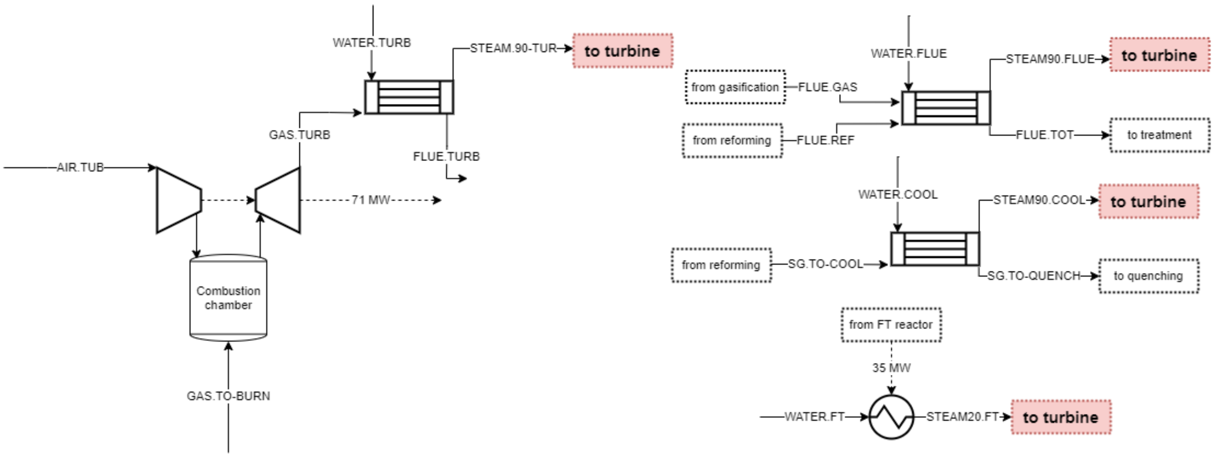

Figure B. 11 - Flowchart for the heat integration/steam generation (LCM GFT)

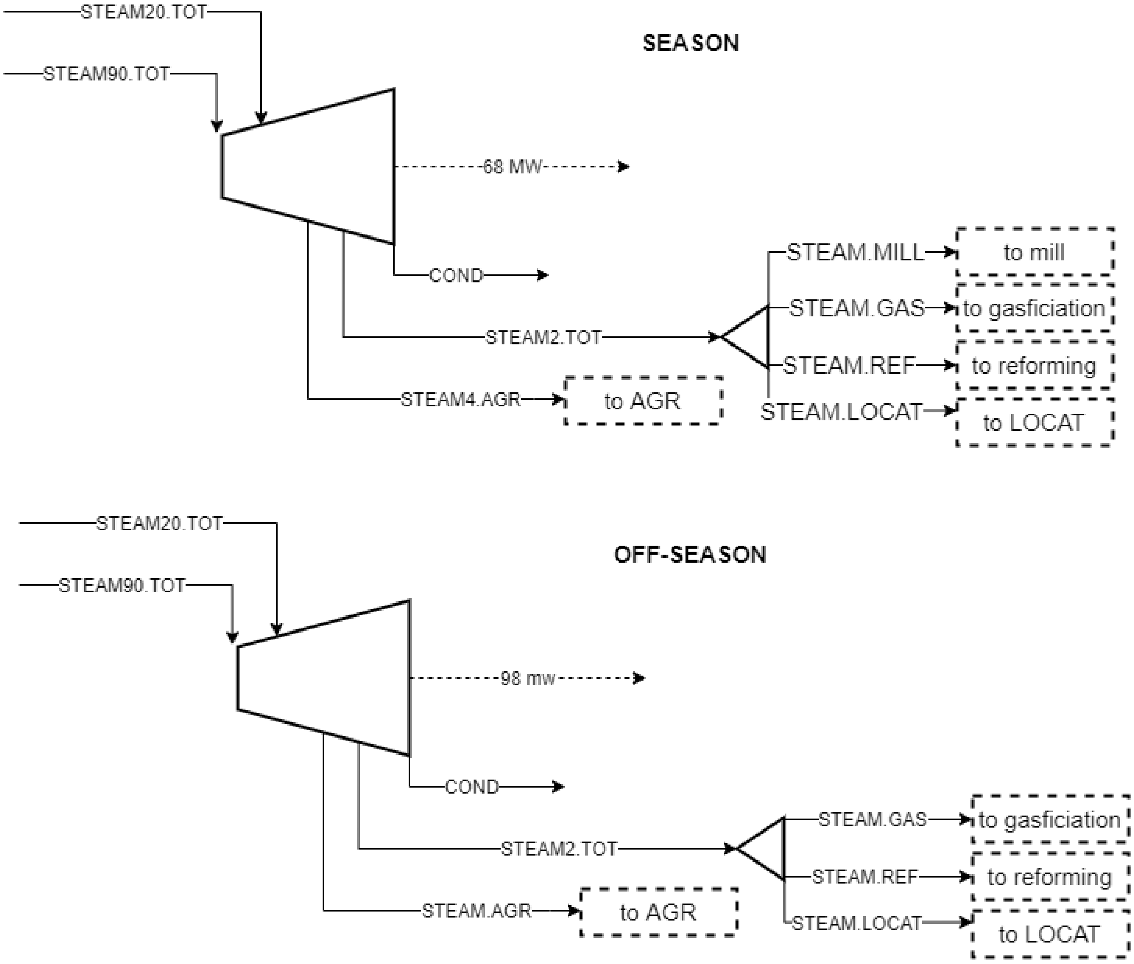

Figure B. 12 - Flowchart for the electricity production/steam generation (LCM GFT)

ii.iii. - GFT route - Scenario 2

The simulation of Scenario 2 follows the same steps as Scenario 1, with the exception of the power and steam generation. Without the 1G mill, the steam and energy requirements for the plant are lower, so a higher fraction of the gases are recycled to the FT reacto (split ratio of 0.8 to SG.REC). Besides that, there is no STEAM.MILL stream. The power generation unit for Scenario 2 is similar with the off-season operation for Scenario 1 (Figure B. 11 and Figure B. 12)

ii.iv. - GFT route - Scenarios 3 and 4

(1) Preprocessing/Gasification/Syngas cleaning

The overall process for bio oil gasification is similar to LCM gasification, with some distinctions:

- There is no required preprocessing of the feedstock;
- Use of a pressurized entrained flow gasifier, operating with pure oxygen (ER = 0.3), and 1200 °C, 25 bar;
- Formation of 2% wt. of soot during gasification [14];
- Cooling of the gases to 500°C, with quenching to clean the gas from the soot;
- Only the AGR and PSA are required for the syngas cleaning. These processes oparete at same conditions as Scenarios 1 and 2;

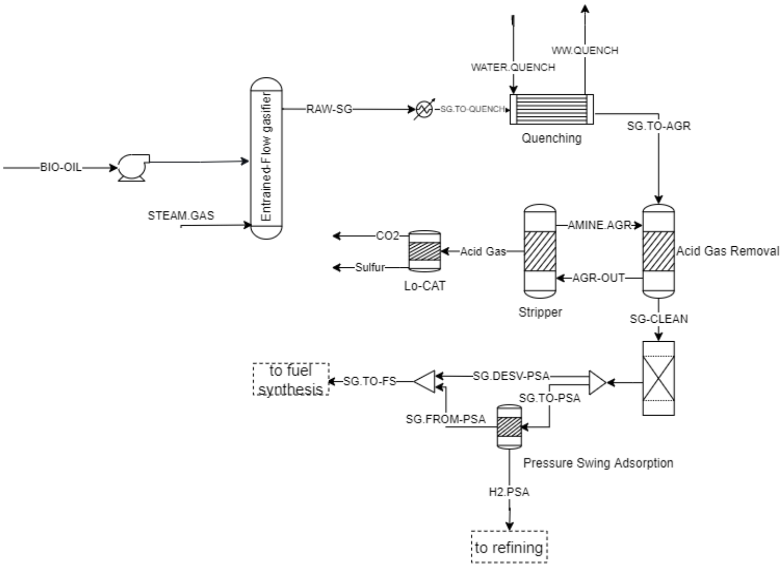

Figure B. 13 - Process flowchart for the production and cleaning of syngas from bio-oil

(2) Fuel synthesis

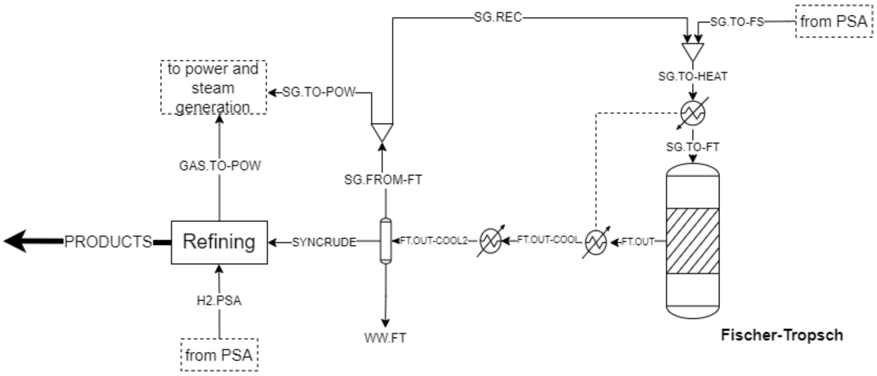

Figure B. 14 - Flowchart for the fuel synthesis processes (bio-oil GFT)

(3) Power and steam generation

The design of the steam and electricity production of the BO GFT plant is similar to the design of Scenario 2, with the exception that there are less “hot streams” to generate steam. For example, since there is no catalyst regenerator (tar reformer), there is not a steam stream associated with this stream, as is the same with a stream from the gasifier combustor.

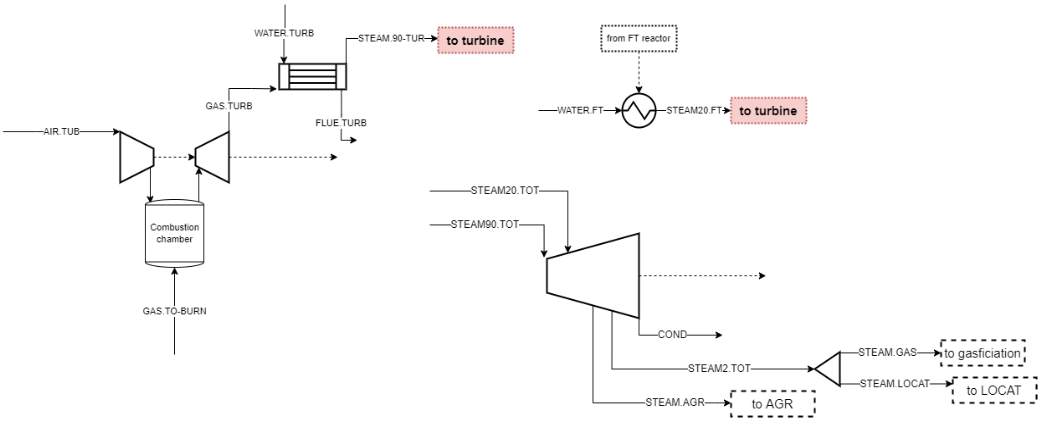

Figure B. 15 - Flowchart for the electricity production/steam generation (bio-oil GFT)

iii. - Logistic aspects

Since the whole purpose of stablishing densification units is to minimize feedstock transportation costs, a logistic evaluation of the proposed route was performed. The VS platform allows the evaluation of logistics related mainly to feedstock collection, transportation and storage, and product transportation. This analysis calculates the costs related to the feedstock transportation to the gasification/F-T plant, and assesses the limitations these costs imply to the biojet production chain. With this platform it is possible to calculate the transportation costs of a given biomass and/or product. However, it is necessary to define the distances related to such transport.

The VSB already has the capacity to calculate the distances related to the collection of biomass for a 1G mill. This allows to determine a mean radius of transportation of biomass from the field to the mill. This radius can be used for the integrated configuration and is dependent mainly on the processing capacity of sugarcane stalks. The VSB then calculates the biomass cost (both for sugarcane stalks and straw).

However, for the distance from the mill to the BtL plant additional considerations are necessary. The VSB is able to calculate the costs of biomass transportation in terms of US$.ton^{-1}km^{-1}, thus it is necessary to determine the transportation distance. First of all, it was considered that 1G mill with annual processing capacity of 2 M tons of sugarcane are selling 100% of their produced LCM to the BtL plant. This capacity was chosen for a base scenario since this is an usual capacity for plants in the Center-East region [15]. The consideration of selling 100% of the LCM is an oversimplification to facilitate these initial estimations, but can also reflect the technological conditions of some mills that are not technologically optimized to export surplus electricity to the grid. Both the capacity of these mills and the amount of LCM they would sell are parameters that can be changed and are part of a sensitivity analysis.

The definition of the profile of these mills help to determine the number of mills necessary to supply the material for the BtL plant. For example, to supply a thermochemical standalone plant processing 1 M tons of dry LCM per year, at least 3 mills with annual milling capacity of 2 M tons of sugarcane are necessary (each plant produces around 0.4 M tons of dry LCM per year). In turn, the number of necessary mills is used to calculate the minimum distance to transport the LCM to the BtL plant.

In order to calculate this distance, some considerations were made. First, it is considered that the distance between the different mill is the minimum possible, such as that the area for each mill – i.e., the sugarcane cropland area of each industrial plant – is tangential to one another without overlap, as can be seen on Figure B. 16.

The second consideration is that these mills are identical in terms of crushingcapacity, technology profile, and percentage of LCM sold. It is also considered that the BtL plant is equidistant from each of the mills.

Figure B. 16 presents a simplified diagram for these considerations, with examples for a cluster with 1 to 4 mills. For cases where only 1 to 2 mills are necessary, the average transportation distance (d) is equal to the mean radius (r) of the mills, which is estimated according to the sugarcane cropland area that is necessary to supplying each mill. For cases with more than 3 mills, such plants are distributed alongside equilateral polygons with edge equal to 2r. For cases with 3 mills, the distribution follows an equilateral triangle with the BtL plant at the center. For 4 plants, this localization follows a square, and so forth. With this in mind, for cases with more than 2 mills, the average distance can be calculated according to Eq. 05.

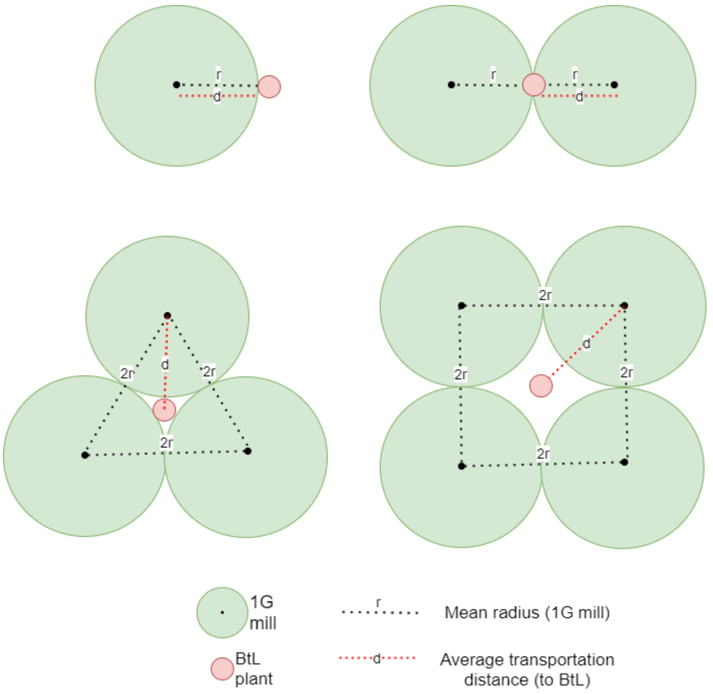

Figure B. 16 - Diagram for estimating the minimum transportation distance from sugarcane mills to the BtL plant

$$d = \frac{r}{cos\left[\frac{(n-2).180}{2.n}\right]} \qquad \text{Eq. B.05}$$

Where d is the transportation distance, r is the mean radius of the mill, and n is the number of required mills.

These considerations are based on a hypothetical scenario with optimal distribution of mills and the BtL plant. For a more realistic scenario, this distance ‘d’ would most likely be larger than the calculated by Eq. 05. With this in mind, besides the profile of each mill, the actual distance can also be a term subject to variations for a sensitivity analysis.

iv. - Life Cycle inventory

Table B. 12 - Life cycle inventory for GFT process – Scenario 1

Materials/fuels/processes	**Value per year**	**Unit**	**Impact (kg CO2 eq/unit)**
Conventional Sugarane	4.00E+09	kg	3.88E-02
Straw wet	3.42E+08	kg	6.67E-03
Quicklime, milled, packed, at plant/CH U	2.55E+06	kg	9.85E-01
Sulphuric acid, liquid, at plant, market mix/CTBE BR U	1.68E+06	kg	1.77E-01
Phosphoric acid, industrial grade, 85% in H2O, at plant/RER U	9.24E+08	g	1.42E-03
Chemicals inorganic, at plant/GLO U	1.06E+07	g	1.86E-03
Chemicals inorganic, at plant/GLO U	3.16E+07	g	1.86E-03
Sand, market for/GLO U	2.15E+04	kg	1.17E-02
Chemicals inorganic, at plant/GLO U	1.30E+08	g	1.86E-03
Zinc oxide {GLO}| market for | Alloc Rec, U	2.19E+01	kg	1.70E+00
Dimethylamine {GLO}| market for	9.42E+04	kg	2.37E+00
Water treatment biorefinery/CTBE BR U	1.34E+09	kg	1.58E-04
Bagasse, to combustion in industrial boiler, dry basis/CTBE BR U	2.05E+08	kg	2.78E-02
Biogas, as CH4, to combustion/CTBE BR U	2.21E+08	kg	1.96E-02
Lubricating oil, market mix/CTBE BR U	5.40E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	5.99E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	3.55E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	8.14E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	1.70E+02	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	1.02E+09	kg	0

Table B. 13 - Life cycle inventory for GFT process – Scenario 2

Materials/fuels/processes	Value per year	Unit	Impact (kg CO2 eq/unit)
Straw wet harvest	2.94E+08	kg	4.97E-03
bagasse wet harvest	9.56E+08	kg	0.00E+00
straw transportation	2.94E+08	kg	2.44E-03
bagasse tranportation	9.56E+08	kg	1.74E-03
Chemicals inorganic, at plant/GLO U	2.48E+07	g	1.86E-03
Sand, market for/GLO U	1.69E+04	kg	1.17E-02
Chemicals inorganic, at plant/GLO U	1.29E+08	g	1.86E-03
Zinc oxide {GLO}| market for | Alloc Rec, U	1.71E+01	kg	1.70E+00
dimethylamine	7.38E+04	kg	2.37E+00
Water treatment biorefinery/CTBE BR U	1.07E+09	kg	1.58E-04
Bagasse, to combustion in industrial boiler, dry basis/CTBE BR U	1.60E+08	kg	2.78E-02
Biogas, as CH4, to combustion/CTBE BR U	1.31E+08	kg	1.96E-02
Lubricating oil, market mix/CTBE BR U	1.29E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	4.78E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	2.83E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	6.49E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	1.36E+02	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	5.47E+08	kg	0.00E+00

Table B. 14 - Life cycle inventory of the standalone FP process

Materials/fuels/processes	**Value per year**	**Unit**	**Impact (kg CO2 eq/unit)**
Straw wet harvest	3.42E+08	kg	4.97E-03
bagasse wet harvest	1.11E+09	kg	0.00E+00
straw transportation	9.45E+06	tkm	9.57E-02
bagasse tranportation	3.08E+07	tkm	6.81E-02
market for methanol, global	4.19E+07	kg	6.38E-01
Bagasse, to combustion in industrial boiler, dry basis/CTBE BR U	2.06E+08	kg	2.78E-02
Biogas, as CH4, to combustion/CTBE BR U	5.55E+08	kg	1.96E-02
Lubricating oil, market mix/CTBE BR U	1.50E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	2.34E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	1.38E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	3.18E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	6.65E+01	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	6.26E+08	kg	0.00E+00

Table B. 15 - Life cycle inventory of the GFT process - Scenario 3

Materials/fuels/processes	**Value per year**	**Unit**	**Impact (kg CO2 eq/unit)**
bio oil	6.99E+08	kg	1.02E-01
bio oil transportation	3.86E+07	tkm	4.44E-02
Water treatment biorefinery/CTBE BR U	1.34E+08	kg	1.58E-04
Biogas, as CH4, to combustion/CTBE BR U	1.43E+08	kg	1.96E-02
Chemicals inorganic, at plant/GLO U	1.51E+08	g	1.86E-03
Zinc oxide {GLO}| market for | Alloc Rec, U	8.68E-01	kg	1.70E+00
dimethylamine	2.78E+05	kg	2.37E+00
Lubricating oil, market mix/CTBE BR U	1.37E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	4.88E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	2.89E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	6.63E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	1.39E+02	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	5.39E+08	kg	0.00E+00

Table B. 16 - Life cycle inventory for the integrated FP process

Materials/fuels/processes	**Value per year**	**Unit**	**Impact (kg CO2 eq/unit)**
Conventional Sugarane/CTBE BR U	4.00E+09	kg	3.88E-02
Straw wet	3.42E+08	kg	6.67E-03
Quicklime, milled, packed, at plant/CH U	2.55E+06	kg	9.85E-01
Sulphuric acid, liquid, at plant, market mix/CTBE BR U	1.68E+06	kg	1.77E-01
Phosphoric acid, industrial grade, 85% in H2O, at plant/RER U	9.24E+08	g	1.42E-03
Chemicals inorganic, at plant/GLO U	1.06E+07	g	1.86E-03
market for methanol, global	4.19E+07	kg	6.38E-01
Water treatment biorefinery/CTBE BR U		kg	1.58E-04
Bagasse, to combustion in industrial boiler, dry basis/CTBE BR U	2.06E+08	kg	2.78E-02
Biogas, as CH4, to combustion/CTBE BR U	5.55E+08	kg	1.96E-02
Lubricating oil, market mix/CTBE BR U	5.40E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	3.53E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	2.09E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	4.79E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	1.00E+02	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	8.81E+08	kg	0.00E+00

Table B. 17 - Life cycle inventory for the GFT process - Scenario 4

Materials/fuels/processes	**Value per year**	**Unit**	**Impact (kg CO2 eq/unit)**
bio oil	6.99E+08	kg	3.05E-01
bio oil transportation	6.99E+08	tkm	4.44E-02
Water treatment biorefinery/CTBE BR U	1.34E+08	kg	1.58E-04
Biogas, as CH4, to combustion/CTBE BR U	1.43E+08	kg	1.96E-02
Chemicals inorganic, at plant/GLO U	1.51E+08	g	1.86E-03
Zinc oxide {GLO}| market for | Alloc Rec, U	8.68E-01	kg	1.70E+00
dimethylamine	2.78E+05	kg	2.37E+00
Lubricating oil, market mix/CTBE BR U	1.37E+07	g	8.78E-04
Steel product manufacturing, average metal working/RER U	4.88E+05	kg	1.79E+00
Chromium steel product manufacturing, average metal working/RER U	2.89E+04	kg	2.43E+00
Concrete, sole plate and foundation, at plant/CH U	6.63E+02	m3	1.60E+02
Building, hall, steel construction/CH/I U	1.39E+02	m2	3.09E+02
Emissions to air			
Carbon dioxide, biogenic	3.91E+08	kg	0.00E+00

v. - Economic estimations

Table B. 18- Main assumptions for the techno-economic assessment

Item	Value	Reference
Expected project lifetime	25 years	(BONOMI et al., 2016)
Discount rate	12% per year	(BONOMI et al., 2016)
Reference date	December 2019	Assumed
Exchange rate	R$ 4.03 = 1 US$	(BANCO CENTRAL DO BRASIL, 2020)
Depreciation	10 years, linear	(BONOMI et al., 2016)
Working capital	10% of CAPEX	(BONOMI et al., 2016)
Taxes	25% + 9% of taxable income	(BONOMI et al., 2016)
Maintenance	3% of CAPEX	(DUTTA et al., 2011)
Insurance and others	0.7% of CAPEX	(DUTTA et al., 2011)
Sugarcane bagasse cost	12 US$/ton	(LEAL and HERNANDES, 2020)
Ethanol price	0.43 US$/L	(CEPEA, 2020)
Biojet fuel price	0.53 US$/L	(ANP, 2020)
Green gasoline price	0.45 US$/L	(ANP, 2020)
Electricity price	US$ 54/MWh	(CCEE, 2020)

Table B. 19 - Equipment purchase and installed costs (Integrated Fast Pyrolysis)

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
1G ethanol plant	-	-	-		-	VSB [1]	-		4	M ton sugarcane/year	-	-			107.49	M US$
LCM preprocessing																
straw reception and processing	-	-	-		-	VSB [1]	-		171089	ton straw/year	-	-			6.2	M US$
Dryer	74	ton evaporated water/h	7.63	M US$	2002	[16]	18.85	M US$	84.6	ton evaporated water/h	1	1.325	17.74	M US$	43.83	M US$
Bio oil production																
Pyrolyzer	500	ton biomass/day	0.836	M US$	2012	[17]	2.52	M US$	2383	ton biomass/day	-	1.325	5.76	M US$	17.38	M US$
Bio oil condenser	109	ton bio oil/h	0.999	M US$	2012	[17]	2.39	M US$	52.94	ton bio oil/h	0.79	1.325	0.78	M US$	2.35	M US$
Storage	1000	m³/month	0.315	M US$	2014		0.73	M US$	3697	m³/month	-	1.325	5.14	M US$	11.87	M US$

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Steam system and power generation																
Water treatment	216.3	ton/h	2.47	M US$	2007	[8]	2.841	M US$	330	ton/h	0.7	1.325	5.08	M US$	5.84	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[8]	1.597	M US$	330	ton/h	0.3	1.325	1.1	M US$	2.7	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.29	M US$	2007	[8]	0.702	M US$	330	ton/h	0.65	1.325	0.48	M US$	1.1	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	34.9	MW	0.7	1	4.43	M US$	7.97	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	12.8	MW	0.7	1	4.3	M US$	7.7	M US$
Boiler	226	ton inlet/h	0.24	M US$	2012	[17]	0.74	M US$	437	ton inlet/h	0.7	1.325			7.49	M US$
Transmission/stations	-	-	-	-	-	-	-	-	67	MW	-	-	-	-	15.15	M US$
Heat integration	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4.32	M US$
Utilities																
Air systems	119	ton biomass/h	0.3	M US$	2007	[8]	0.57	M US$	390	ton biomass/h	0.3	1.325	0.66	M US$	1.25	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[8]	1.909	M US$	383	ton flue gas/h	0.65	1.325	1.19	M US$	2.73	M US$

Table B. 20 - Inputs costs (FP process, standalone)

Variable Operating Costs	**Reference cost**		**Ref.**	**Year**	**Value**		**Total cost**	
Methanol	0.296	US$/kg	[18]	Dez/19	41925191	kg/year	12.42	MUS$/year
Chemicals for water system	0.0327	US$/m3	[1]	Dez/17	6.70E+05	M³/year	0.02	MUS$/yea
Steam system	0.035	US$/ton Steam	[1]	Dez/17	6.17E+06	Ton/year	0.22	M US$/year

Table B. 21 - Equipment purchase and installed costs (Standalone Fast Pyrolysis)

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
LCM preprocessing																
straw reception and processing	-	-	-		-	VSB [1]	-		171089	ton straw/year	-	-			6.2	M US$
Dryer	74	ton evaporated water/h	7.63	M US$	2002	[16]	18.85	M US$	84.6	ton evaporated water/h	1	1.325	17.74	M US$	43.83	M US$
Bio oil production																
Pyrolyzer	500	ton biomass/day	0.836	M US$	2012	[17]	2.52	M US$	2383	ton biomass/day	-	1.325	5.76	M US$	17.38	M US$
Bio oil condenser	109	ton bio oil/h	0.999	M US$	2012	[17]	2.39	M US$	52.94	ton bio oil/h	0.79	1.325	0.78	M US$	2.35	M US$
Storage	1000	m³/month	0.315	M US$	2014		0.73	M US$	3697	m³/month	-	1.325	5.14	M US$	11.87	M US$

	Capacity (base)		Equipment cost		Year	Ref	Installed Cost (base)		Scalled capacity		Scale factor	Local. Factor	Equipment cost	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit
Steam system and power generation														
Water treatment	216.3	ton/h	2.47	M US$	2007	[8]	2.841	M US$	330	ton/h	0.7	1.325	5.08	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[8]	1.597	M US$	330	ton/h	0.3	1.325	1.78	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	34	MW	0.7	1	4.4	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	48	MW	0.7	1	10.8	M US$
Boiler	226	ton inlet/h	0.24	M US$	2012	[17]	0.74	M US$	437	ton inlet/h	0.7	1.325		
Transmission/stations	-	-	-	-	-	-	-	-	67	MW	-	-	-	-
Heat integration	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Utilities														
Air systems	119	ton biomass/h	0.3	M US$	2007	[8]	0.57	M US$	390	ton biomass/h	0.3	1.325	0.66	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[8]	1.909	M US$	383	ton flue gas/h	0.65	1.325	1.19	M US$

Table B. 22 - Inputs costs (FP process, integrated)

Variable	Reference cost		Ref.	Year	Value		Total cost	
Operating Costs								
Mill chemicals inputs	-	-	VSB [1]	2019	-	-	1.25	M US$/year
Other mill inputs cost	-	-	VSB [1]	2019	-	-	1.03	M US$/year
Methanol	0.296	US$/kg	[18]	Dez/19	41925191	kg/year	12.42	MUS$/year
Chemicals for water system	0.0327	US$/m3	[1]	Dez/17	6.70E+05	M³/year	0.02	MUS$/yea
Steam system	0.035	US$/ton Steam	[1]	Dez/17	6.17E+06	Ton/year	0.22	M US$/year

Table B. 23 - Equipment purchase and installed costs of GFT process (Scenario 1)

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
1G ethanol plant	-	-	-		-	VSB [1]	-		4	M ton sugarcane/year	-	-			107.49	M US$
LCM preprocessing																
straw reception and processing	-	-	-		-	VSB [1]	-		349703.77	ton straw/year	-	-			9.53	M US$
Dryer	74	ton evaporated water/h	7.63	M US$	2002	[16]	18.85	M US$	73.68	ton evaporated water/h	1	1.325	15.45	M US$	38.17	M US$
Syngas production																
Gasification + Tar reformer	68.55	ton biomass (d.b)/h	19.8	M US$	2010	[8]	45.74	M US$	102.82	ton biomass (d.b)/h	1	1.325	48.75	M US$	112.61	M US$
heat integration*						[8]									4.03	M US$
compression	28.934	MW (energy consumption)	16.81	M US$	2005	[11]	41.521	M US$	24.14	MW (energy consumption)	0.62	1.325	25.82	M US$	63.78	M US$
AGR	66.38	ton acid gas/h	6.79	M US$	2007	[4]	20.37	M US$	57.49	ton acid gas/h	0.75	1.325	9.34	M US$	28.02	M US$
Sulfur recovery	0.042	ton sulfur/h	2.92	M US$	2002	[8]	3.942	M US$	0.04	ton sulfur/h	0.75	1.325	4.68	M US$	6.31	M US$
Fuel synthesis																
FT reactor	100	MW (FT liquids)			2000	[12]	16.7	M US$	100	MW (FT liquids)	1	1.325			28.77	M US$
other	113.7	ton syngas/h	4.51	M US$	2007	[4]	4.51	M US$	71.2	ton syngas/h	1	1.325	0.8	M US$	0.8	M US$
Hydroprocessing	0.159	m³ liquid fuels/day	0.004	M US$	2007	[19]	0.009	M US$	238.36	m³ liquid fuels/day	1	1.325	9.19	M US$	21.22	M US$
Storage	1000	m³ liquid fuels/month	0.3147	M US$	2014		0.727	M US$	4716.66	m³ liquid fuels/month	1	1.325	2.088	M US$	4.823	M US$

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Steam system and power generation																
Water treatment	216.3	ton/h	2.47	M US$	2007	[8]	2.841	M US$	347	ton/h	0.7	1.325	5.27	M US$	6.06	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[8]	1.597	M US$	347	ton/h	0.3	1.325	1.17	M US$	2.831	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.29	M US$	2007	[8]	0.702	M US$	347	ton/h	0.65	1.325	0.49	M US$	1.186	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	31.9	MW	0.7	1	4.18	M US$	7.52	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	65.94	MW	0.7	1	13.5	M US$	24.26	M US$
Gas turbine	-	-	-	-	-	-	-	-	71.13	MW	-	-	-	-	35.61	M US$
Transmission/stations	-	-	-	-	-	-	-	-	141.74	MW	-	-	-	-	19.65	M US$
Heat integration	-	-	-	-	-	-	-	-	-	-	-	-	-	-	6.88	M US$
Utilities																
Air systems	119	ton biomass/h	0.3	M US$	2007	[8]	0.57	M US$	187.93	ton biomass/h	0.3	1.325	0.53	M US$	1	M US$
Cooling water systems	2660	ton water/h	0.66	M US$	2007	[8]	1.478	M US$	5681.91298	ton water/h	0.6	1.325	1.59	M US$	3.57	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[8]	1.909	M US$	303.79	ton flue gas/h	0.65	1.325	1.02	M US$	2.35	M US$
Purge water treatment	0.1	ton water/h	0.36	M US$	2007	[8]	0.9	M US$	0.21	ton water/h	0.65	1.325	0.89	M US$	2.22	M US$
Chemicals storage	119	ton biomass/h	0.5	M US$	2007	[8]	0.98	M US$	187.93	ton biomass/h	0.65	1.325	1.03	M US$	2.02	M US$

Table B. 24 - Inputs costs (GFT process, Scenario 1)

Variable Operating Costs	Reference cost		Ref.	Year	Value		Total cost	
Mill chemicals inputs	-	-	VSB [1]	2019	-	-	1.25	M US$/year
Other mill inputs cost	-	-	VSB [1]	2019	-	-	1.03	M US$/year
LO-CAT Chemicals	176	US$/ton of S produced	[4]	2007	351.8	ton of S/year	0.09	M US$/year
DEA make-up	2.06	US$/kg	[18]	2019	96286.9	kg amine/year	0.2	M US$/year
Hydroprocessing	11.35	$/m3 produced	[19]	2007	78659.1	m3/year	1.33	M US$/year
FT Catalyst (Cobalt)	33.07	US$/kg	[4]	2007	100.9	ton/year	4.96	M US$/year
Tar reformer catalyst	65.48	US$/kg	[8]	2007	0.0041	ton/h	1.91	M US$/year
Olivine	172.9	US$/ton	[8]	2004	21987.8	kg/year	8.36	M US$/year
ZnO Guard Bed	12536.64	US$/m3	[11]	2005	12.3	m^3/year	0.3	M US$/year
PSA Packing	65180.33	US$/hourly ton syngas in/year	[4]	2007	0.7	ton/h	0.07	M US$/year
Chemicals for water System	0.03	US$/m3	VSB [1]	2017	1318892.9	m3/year	0.04	M US$/year
Steam system	0.03	US$/ton steam	VSB [1]	2017	2705336.4	ton/h	0.09	M US$/year

Table B. 25 - Equipment purchase and installed costs of the GFT process (Scenario 2

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipmen**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	u
LCM preprocessing														
straw reception and processing	-	-	-		-	VSB [1]	-		293546	ton straw/year	-	-		
Dryer	74	ton evaporated water/h	7.63	M US$	2002	[16]	18.85	M US$	62.68	ton evaporated water/h	1	1.325	13.15	M
Syngas production														
Gasification + Tar reformer	68.55	ton biomass (d.b)/h	19.8	M US$	2010	[8]	45.74	M US$	78.88	ton biomass (d.b)/h	1	1.325		
heat integration*						[8]								
compression	28.934	MW (energy consumption)	16.81	M US$	2005	[11]	41.521	M US$	18.52	MW (energy consumption)	0.62	1.325		M
AGR	66.38	ton acid gas/h	6.79	M US$	2007	[4]	20.37	M US$	44.09	ton acid gas/h	0.75	1.325		M
Sulfur recovery	0.042	ton sulfur/h	2.92	M US$	2002	[8]	3.942	M US$	0.03	ton sulfur/h	0.75	1.325		M
Fuel synthesis														
FT reactor	100	MW (FT liquids)			2000	[12]	16.7	M US$	124	MW (FT liquids)	1	1.325		
other	113.7	ton syngas/h	4.51	M US$	2007	[4]	4.51	M US$	104	ton syngas/h	1	1.325		M
Hydroprocessing	0.159	m³ liquid fuels/day	0.004	M US$	2007	[19]	0.009	M US$	304.6	m³ liquid fuels/day	1	1.325		M
Storage	1000	m³ liquid fuels/month	0.3147	M US$	2014		0.727	M US$	6027	m³ liquid fuels/month	1	1.325		M

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Steam system and power generation																
Water treatment	216.3	ton/h	2.47	M US$	2007	[8]	2.841	M US$	265	ton/h	0.7	1.325		M US$	5.01	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[8]	1.597	M US$	265	ton/h	0.3	1.325		M US$	8.47	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	26.69	MW	0.7	1		M US$	6.64	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	32.17	MW	0.7	1		M US$	14.68	M US$
Gas turbine	-	-	-	-	-	-	-	-	29.15	MW	-	-		-	14.6	M US$
Transmission/stations	-	-	-	-	-	-	-	-	66.72	MW	-	-		-	15.11	M US$
Heat integration	-	-	-	-	-	-	-	-		-	-	-		-	4.97	M US$
Utilities																
Air systems	119	ton biomass/h	0.3	M US$	2007	[8]	0.57	M US$	150.33	ton biomass/h	0.3	1.325		M US$	0.94	M US$
Cooling water systems	2660	ton water/h	0.66	M US$	2007	[8]	1.478	M US$	8160	ton water/h	0.6	1.325		M US$	4.44	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[8]	1.909	M US$	236	ton flue gas/h	0.65	1.325		M US$	2.00	M US$
Purge water treatment	0.1	ton water/h	0.36	M US$	2007	[8]	0.9	M US$	0.16	ton water/h	0.65	1.325		M US$	1.89	M US$
Chemicals storage	119	ton biomass/h	0.5	M US$	2007	[8]	0.98	M US$	150.33	ton biomass/h	0.65	1.325		M US$	1.75	M US$

Table B. 26 - Inputs costs (GFT process, Scenario 2)

Variable Operating Costs	Reference cost		Ref.	Year	Value		Total cost	
LO-CAT Chemicals	176	US$/ton of S produced	[4]	2007	270	ton of S/year	70634.50	M US$/year
DEA make-up	2.06	US$/kg	[18]	2019	73846	kg amine/year	151859.51	M US$/year
Hydroprocessing	11.35	$/m3 produced	[19]	2007	100518	m3/year	1696924.98	M US$/year
FT Catalyst (Cobalt)	33.07	US$/kg	[4]	2007	129	ton/year	6358357.02	M US$/year
Tar reformer catalyst	65.48	US$/kg	[8]	2007	0.003	ton/h	1462033.69	M US$/year
Olivine	172.9	US$/ton	[8]	2004	16868	kg/year	6415352.02	M US$/year
ZnO Guard Bed	12536.64	US$/m3	[11]	2005	9.5	m^3/year	231864.78	M US$/year
PSA Packing	65180.33	US$/hourly ton syngas in/year	[4]	2007	0.88	ton/h	85454.59	M US$/year
Chemicals for water System	0.03	US$/m3	VSB [1]	2017	1.07E6	m3/year	35015.03	M US$/year
Steam system	0.03	US$/ton steam	VSB [1]	2017	2.06E6	ton/h	71869.33	M US$/year

Table B. 27 - Equipment purchase and installed costs (GFT Scenarios 3 and 4)

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Syngas production																
Gasification + Tar reformer	68.55	ton biomass (d.b)/h	19.8	M US$	2010	[8]	45.74	M US$	78.88	ton biomass (d.b)/h	1	1.325			75.35	M US$
heat integration*						[8]									2.6	M US$
compression	28.934	MW (energy consumption)	16.81	M US$	2005	[11]	41.521	M US$	18.52	MW (energy consumption)	0.62	1.325		M US$	54.12	M US$
AGR	66.38	ton acid gas/h	6.79	M US$	2007	[4]	20.37	M US$	44.09	ton acid gas/h	0.75	1.325		M US$	22.96	M US$
Sulfur recovery	0.042	ton sulfur/h	2.92	M US$	2002	[8]	3.942	M US$	0.03	ton sulfur/h	0.75	1.325		M US$	5.17	M US$
Fuel synthesis																
FT reactor	100	MW (FT liquids)			2000	[12]	16.7	M US$	124	MW (FT liquids)	1	1.325			35.75	M US$
other	113.7	ton syngas/h	4.51	M US$	2007	[4]	4.51	M US$	104	ton syngas/h	1	1.325		M US$	1.18	M US$
Hydroprocessing	0.159	m^3 liquid fuels/day	0.004	M US$	2007	[19]	0.009	M US$	304.6	m^3 liquid fuels/day	1	1.325		M US$	27.12	M US$
Storage	1000	m^3 liquid fuels/month	0.3147	M US$	2014		0.727	M US$	6027	m^3 liquid fuels/month	1	1.325		M US$	5.47	M US$

	Capacity (base)		**Equipment cost**		**Year**	**Ref**	**Installed Cost (base)**		**Scalled capacity**		**Scale factor**	**Local. Factor**	**Equipment cost**		**Installed Cost (base)**	
Area	Value	unit	Value	unit			Value	unit	Value	unit			Value	unit	Value	unit
Steam system and power generation																
Water treatment	216.3	ton/h	2.47	M US$	2007	[8]	2.841	M US$	265	ton/h	0.7	1.325		M US$	5.01	M US$
Boiler Feed Water/Steam/ Condensate Handling	216.3	ton/h	0.66	M US$	2007	[8]	1.597	M US$	265	ton/h	0.3	1.325		M US$	8.47	M US$
Counter Pressure turbines	44	MW	13.15	M R$	2011	VSB [1]	23.67	M R$	26.69	MW	0.7	1		M US$	6.64	M US$
Condensation/extraction turbines	44	MW	25.5	M R$	2011	VSB[1]	45.9	M R$	32.17	MW	0.7	1		M US$	14.68	M US$
Gas turbine	-	-	-	-	-	-	-	-	29.15	MW	-	-		-	14.6	M US$
Transmission/stations	-	-	-	-	-	-	-	-	66.72	MW	-	-		-	15.11	M US$
Heat integration	-	-	-	-	-	-	-	-		-	-	-		-	4.97	M US$
Utilities																
Air systems	119	ton biomass/h	0.3	M US$	2007	[8]	0.57	M US$	150.33	ton biomass/h	0.3	1.325		M US$	0.94	M US$
Cooling water systems	2660	ton water/h	0.66	M US$	2007	[8]	1.478	M US$	8160	ton water/h	0.6	1.325		M US$	4.44	M US$
Flue gas treatment	425.7	ton flue gas/h	0.83	M US$	2007	[8]	1.909	M US$	236	ton flue gas/h	0.65	1.325		M US$	2.00	M US$
Purge water treatment	0.1	ton water/h	0.36	M US$	2007	[8]	0.9	M US$	0.16	ton water/h	0.65	1.325		M US$	1.89	M US$
Chemicals storage	119	ton biomass/h	0.5	M US$	2007	[8]	0.98	M US$	150.33	ton biomass/h	0.65	1.325		M US$	1.75	M US$

Table B. 28 - Inputs costs (GFT, Scenarios 3 and 4)

Variable Operating Costs	**Reference cost**		**Ref.**	**Year**	**Value**		**Total cost**	
LO-CAT Chemicals	176	US$/ton of S produced	[4]	2007	128.15	ton of S/year	0.034	M US$/year
DEA make-up	2.06	US$/kg	[18]	2019	278261.25	kg amine/year	0.572	M US$/year
Hydroprocessing	11.35	$/m3 produced	[19]	2007	122193.61	m3/year	2.063	M US$/year
FT Catalyst (Cobalt)	33.07	US$/kg	[4]	2007	151.11	ton/year	7.431	M US$/year
ZnO Guard Bed	12536.64	US$/m3	[11]	2005	0.479	m³/year	0.012	M US$/year
PSA Packing	65180.33	US$/hourly ton syngas in/year	[4]	2007	0.96	ton/h	0.093	M US$/year
Chemicals for water System	0.03	US$/m3	VSB [1]	2017	1.34E+05	m3/year	0.004	M US$/year
Steam system	0.03	US$/ton steam	VSB [1]	2017	1.83E+06	ton/h	0.06	M US$/year

vi. - Additional results

Table B. 29 - Additional economic and environmental results for Fast pyrolysis

	Standalone	**Integrated**	
CAPEX	179.78	271.06	M US$
OPEX	43.70	122.57	M US$/year
NPV	0.00	87.62 (0 – 404)	M US$
TIR	12%	16% (12 – 27)	per year
NPV/CAPEX	0.00	0.32 (0 – 1.37)	-
Bio-oil minimum selling price	123 (81-164)	70 (33-156)	US$/ton
Bio-oil production costs	123 (81-164)	63 (28-155)	US$/ton
capital	*44.94*	*14.55*	
biomass purchase	*38.84*	*37.85*	
biomass transportation	*1.42*	*0.00*	
Other inputs costs	*22.87*	*5.90*	
Other O&M costs	*15.81*	*4.80*	
Capacity	0.73	0.73	M ton LCM/year d.b
	-	4.00	M ton SC/year
Products	0.42	0.42	M ton/year
Total emissions	0.05	0.23	M ton $CO_{2\ eq}$/year

Table B. 30 - Additional economic and environmental results for the GFT scenarios

	Scenario 1	**Scenario 2**	**Scenario 3**	**Scenario 4**	
CAPEX	566	367	375	375	M US$
OPEX	142	51	121	79	M US$/year
NPV	-36 (-320 – 220)	-181 (-388 – -78)	-679 (-920 - -479)	-448 (-860 - -248)	M US$
TIR	11% (4 – 17)	4% (-4 – 9)	-	-	per year
NPV/CAPEX	-0.06 (-0.48 – 0.40)	-0.49 (-0.86 - -0.23)	-1.81 (-2.24 - -1.27)	-1.2 (-2.07 - -0.67)	-
Jet Fuel production costs	0.54 (0.39 – 0.73)	0.78 (0.61 – 1.00)	1.54 (1.23 – 1.91)	1.23 (0.91 – 1.79)	US$/L
capital	0.18	0.34	0.44	0.45	
feedstock purchase	0.24	0.15	0.84	0.51	
feedstock transportation	0.00	0.01	0.02	0.01	
Other inputs costs	0.05	0.14	0.09	0.10	
Other O&M costs	0.06	0.13	0.14	0.16	
Capacity	0.80	0.62	-	-	M ton LCM/year d.b
	4	-	-	-	M ton SC/year
	-	-	0.70	0.70	M ton BO/year
Products	$3.8.10^9$	$3.8.10^9$	$3.8.10^9$	$3.8.10^9$	MJ liquid fuels/year

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Annex C - Authorization for using the published papers

Bottlenecks and potentials for the gasification of lignocellulosic biomasses and Fischer-Tropsch synthesis: A case study on the production of advanced liquid biofuels in Brazil

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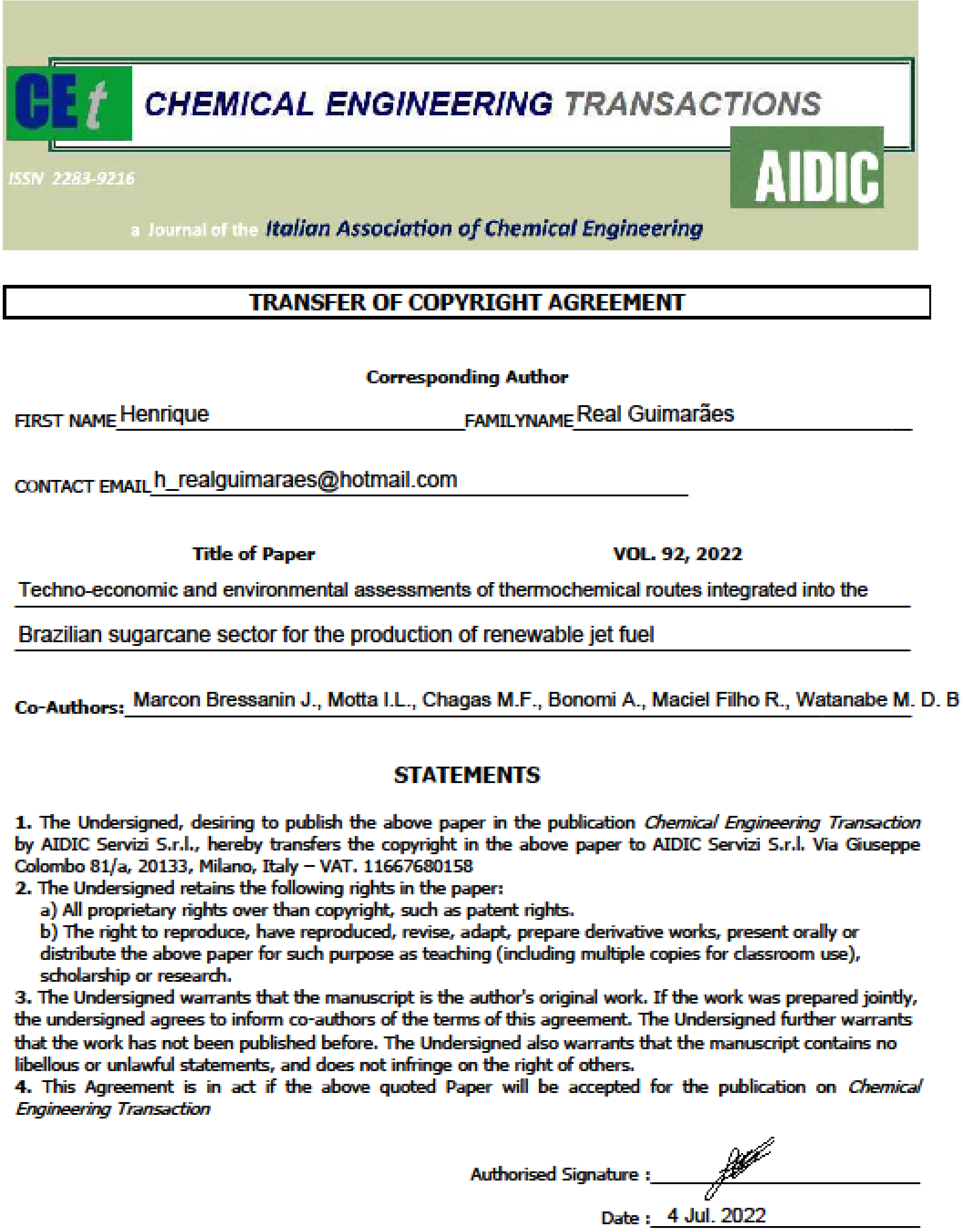

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Title of Paper **VOL. 92, 2022**

Techno-economic and environmental assessments of thermochemical routes integrated into the Brazilian sugarcane sector for the production of renewable jet fuel

Co-Authors: Marcon Bressanin J., Motta I.L., Chagas M.F., Bonomi A., Maciel Filho R., Watanabe M. D. B

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Decentralization of sustainable aviation fuel production in Brazil through Biomass-to-Liquids routes: A techno-economic and environmental evaluation

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