

Sugestões de Alteração do fator de intensidade de carbono para o bioquerosene na Proposta de Metas do RenovaBio do MME

A atribuição de um fator de intensidade de carbono para o bioquerosene, rota HEFA, é mais elevado do que o esperado (34,65 gCO₂/MJ). Na apresentação “Explorando a Renovacalc” (Figura 1) no evento “Bioquerosene e Renovabio”, ficou claro que utilizou-se hidrogênio oriundo do processo de eletrólise da água como fonte de geração de H₂. Ocorre que esse processo é muito intensivo em eletricidade, o que faz a pegada de carbono disparar.

Na verdade, mais de 90% do H₂ gerado no mundo ocorre através de outro processo, a reforma a vapor de gás natural. Apesar de utilizar combustível fóssil (gás natural) esse é o processo mais competitivo e com menor pegada de carbono do que a eletrólise. De fato, a literatura mostra [1] que a redução de emissões de gases de efeito estufa é da ordem de 70% no bioquerosene rota HEFA comparado ao QAV fóssil. Nesse caso, o valor de 34,65 gCO₂/MJ cairia para cerca de 26,3 gCO₂/MJ, o que é muito parecido com o biodiesel.

Algumas publicações apontam valores da produção de Bioqav HEFA a partir de soja uma emissão de 16,9 gCO₂/MJ (H₂ a partir de eletrolise de água - WE), emissão de 29,2 gCO₂/MJ (H₂ a partir de reforma catalítica de vapor de etanol - CESR) e emissão de 22,5 gCO₂/MJ (H₂ a partir de gás natural, com biomassa palma)

Isso faz sentido?

Sim, pois partindo-se do mesmo óleo vegetal, o biodiesel é produzido pela reação do óleo com metanol, enquanto que o bioquerosene reage óleo com H₂. É bom lembrar que toda a geração de metanol ocorre através de uma primeira etapa de reforma a vapor do gás natural, gerando CO e H₂. Numa segunda etapa do processo, CO e H₂ são convertidos em metanol. Portanto o H₂ é um intermediário na geração de metanol. Portanto, faz sentido um processo que utiliza H₂ (bioquerosene) ter uma pegada de carbono similar a um processo que utiliza metanol (biodiesel).

Essa alteração é bastante importante pois esses dados de intensidade de carbono alimentam a Modelagem do Renovabio que prevê volumes de bioquerosene bem como impactos no preço.

Portanto, solicita-se uma alteração da intensidade de carbono do bioquerosene para algo próximo de 26,7 gCO₂/MJ.

O que contribui para os impactos do bioquerosene?

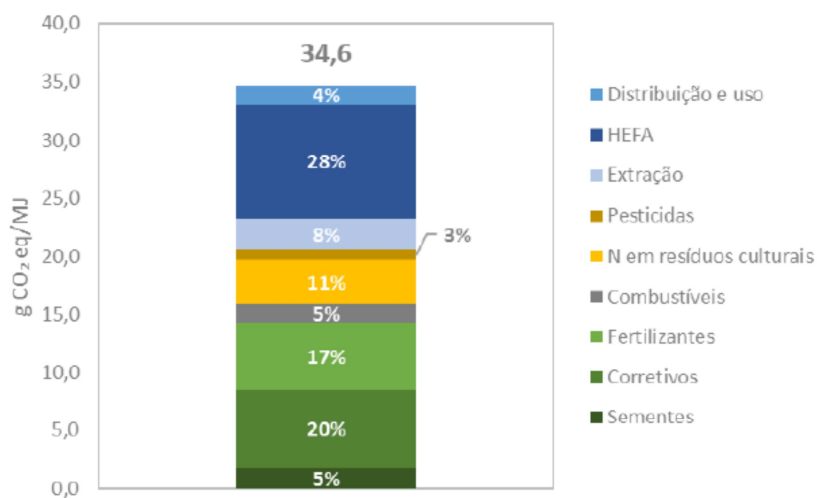


Figura 1 – Slide da Apresentação “Explorando a Renovacalc” no evento “Bioquerosene e Renovabio”, observa-se que boa parte da pegada de carbono deve-se ao processo HEFA, pela consideração de uso de hidrogênio proveniente de eletrólise da água (intensivo em eletricidade).

Outras comparações de LCA:

Pathway	GHG emissions (gCO ₂ e/MJ)
Baseline	89.0
SIP (Sugarcane)	50.6*
HEFA (FOG)	22.5
HEFA (PFAD)	20.7
FT (MSW)	40
ATJ via. iBuOH (Corn)	75*

*These will depend on the calculation of a land use change emissions factor, which is still a work in progress.

Table E1. Comprehensive table with main outcomes of the assessed biorefineries

Biojet fuel route	Biojet fuel feedstock	H ₂ production	5% jet fuel substitution target *	# plants to at least 5% target	CAPEX for at least 5% target (R\$ billion)	Total agricultural land to at least 5% target (thousand ha)	IRR of the biorefinery **	Production			GHG emissions *** (g CO ₂ eq/MJ jet fuel)
								Diesel (million L/yr)	Ethanol (million L/yr)	Electrical energy (GWh/yr)	
HEFA	Palm	WE	71%	2	4.3	348	3.7%	122	360	0	22.3
HEFA	Macacuba	WE	69%	2	4.2	250	9.2%	118	360	0	17.3
HEFA	Soybean	WE	61%	2	4.0	1,332	3.6%	105	360	0	16.9
ATJ	Isobutanol	WE	43%	3	3.5	158	5.7%	4	0	631	17.7
HEFA	Palm	CESR	38%	3	4.7	351	NC	65	0	630	34.5
ATJ	1G2G Ethanol	WE	37%	3	4.7	158	NC	11	0	0	24.8
HEFA	Macacuba	CESR	37%	3	4.7	273	NC	63	0	637	28.7
HEFA	Soybean	CESR	33%	3	4.6	1,170	NC	57	0	649	29.2
ATJ	1G Ethanol	WE	28%	4	4.2	211	0.6%	8	0	525	20.7
FT	Sugarcane+Eucalyptus	Gasification	27%	4	8.0	341	13.5%	81	360	45	9.3
ATJ	1G Ethanol	CESR	20%	5	5.0	263	NC	6	0	657	24.5
FT	Sugarcane	Gasification	11%	9	12.0	474	16.5%	33	360	156	9.4

* Substitution of 5% of the Brazilian fossil jet fuel consumption in 2014, equivalent to 375 million L/yr

** Values shown as NC indicate non-calculated IRR (revenues lower than expenses)

*** For comparison, GHG emissions of conventional, fossil jet fuel: 83.6 g CO₂ eq/MJ jet fuel)

Abbreviations

ATJ: Alcohol to Jet

CESR: catalytic ethanol steam reforming

CAPEX: capital expenditures

FT: Gasification and Fischer-Tropsch Synthesis

WE: water electrolysis

GHG: greenhouse gas

HEFA: Hydroprocessed Esters and Fatty Acids

IRR: Internal Rate of Return

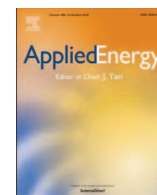
Referência:

- (1) Kadambari Lokesh*, Vishal Sethi, Theoklis Nikolaidis, Eric Goodger, Devaiah Nalianda, "Life cycle greenhouse gas analysis of biojet fuels with a technical investigation into their impact on jet engine performance" Biomass and Bioenergy 77 (2015) 26-44



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Techno-economic and environmental assessment of renewable jet fuel production in integrated Brazilian sugarcane biorefineries



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HIGHLIGHTS

- Integrated biorefineries for year-round production of renewable jet fuel (RJF).
- Assessment of three RJF production routes with ASTM approval.
- On-site H₂ production via water electrolysis with bioelectricity from sugarcane.
- HEFA with highest RJF production potential, while FT with best economic indices.
- RJF with > 70% reduction in greenhouse gas emissions in relation to fossil jet fuel.

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ABSTRACT

The use of renewable jet fuel (RJF) in substitution to fossil jet fuel is one of the main initiatives towards the reduction of impacts derived from carbon emissions by airline operations. This study compares different routes for RJF production integrated with sugarcane biorefineries in Brazil. Eight scenarios with sugarcane mills annexed to three ASTM-approved RJF production technologies, i.e. Hydroprocessed Esters and Fatty Acids (HEFA), Fischer-Tropsch Synthesis (FT), and Alcohol to Jet (ATJ), were assessed. Host mills were considered to crush four million tonnes of sugarcane/year and recover straw from the field. In the designed scenarios, HEFA routes processed palm, macauba, or soybean oils, while FT conversion was based on gasification of either sugarcane or eucalyptus lignocellulosic material, and ATJ converted isobutanol or ethanol into RJF. The biorefineries were assessed in terms of both economic and environmental performance, as well as towards their capability of substituting 5% of the consumption of jet fuel in Brazil in 2014 (equivalent to 375 million L/year). Considering the evaluated scenarios, HEFA-based biorefineries yielded the highest RJF production capacities: a single plant processing palm oil could supply 267 million L RJF/year (71% of the defined target). FT biorefineries presented the best economic performances, producing RJF at competitive cost but with a relatively low output. Finally, all conversion technologies were capable of producing RJF with low climate change impacts, with reductions of over 70% when benchmarked against fossil jet fuel. Carbon mitigation targets of the Brazilian aviation sector are further explored in this paper, showing the dimension of the effort in the coming years for fossil jet fuel replacement in commercial flights. The availability of sugarcane and other biomasses in the country makes Brazil a potentially important player for the deployment of large-scale projects with reasonable RJF market prices and reduced CO₂ emissions for both internal and external markets.

1. Introduction

Most scientists around the world agree that climate change is real and that anthropogenic greenhouse gases (GHG) emissions are at the

root of this issue. According to recent estimates, airline operations were responsible for 2% of such carbon emissions in 2012 [1]. Among actions established by the aviation sector towards lowering the carbon footprint of the sector, three measures initially set for international

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flights within the Carbon Offsetting and Reduction Scheme for International Aviation (CORSIA) mechanism stand out: (1) improving fleet fuel efficiency by 1.5% per year until 2020; (2) stabilizing emissions from 2020 onwards through carbon-neutral expansion; and (3) halving carbon emissions in 2050 in comparison to 2005 levels [2]. Since turbines and aircrafts are already highly efficient [3] and 80% of the emissions come from long-haul flights (which cannot be replaced by alternative transport options) [2], the bulk of the transition will come from the adoption of low-carbon jet fuel derived from biomass.

Conventional jet fuels, usually commercialized under A/A-1 (civil) and JP-8 (military) grades, are produced from crude oil, although ASTM International and other standards organizations also specify the synthesis of alternative jet fuels. Four of the five currently approved routes produce alternative jet fuel exclusively composed of paraffinic hydrocarbons (linear, branched, and cyclic), denominated Synthesized Paraffinic Kerosene (SPK). For use in turbines, SPK must be blended with fossil jet fuel in proportions ranging from 10% to 50%, depending on the conversion route used to obtain it [4]. A single pathway for the production of alternative jet fuels comprising both paraffinic and aromatic compounds, denominated Synthesized Paraffinic Kerosene plus Aromatics (SKA), is also permitted by the organization. Although the mixing of SKA with conventional jet fuel up to 50% is mandatory, such routes tend to focus its application at a longer time horizon. Since this type of jet fuel presents a more similar composition to its fossil counterpart, it could theoretically dismiss blend requirements. In short, the five conversion routes approved by ASTM International (as of September 2017) are: Hydroprocessed Esters and Fatty Acids (HEFA-SPK), which processes vegetable oils and animal fats into hydrocarbons; Fischer-Tropsch Synthesis (both FT-SPK and FT-SKA), in which different feedstocks undergo gasification and further catalytic synthesis to a wide range of hydrocarbons; Alcohol to Jet (ATJ-SPK), which converts isobutanol (and, potentially, other alcohols) into hydrocarbons; and Synthesized Isoparaffins (SIP-SPK), which produces jet fuel-like molecules through fermentation of carbohydrates [4]. Feedstocks for alternative jet fuels include either fossil resources, such as coal, natural gas, and shale oil, or biomass, in the form of lignocellulosic material, lipids, alcohols, and simple carbohydrates. For the remainder of this study, only alternative jet fuels obtained from biobased feedstocks are considered, henceforth referred to as renewable jet fuel (RJF).

The employment of RJF in civil aviation appears to be the best short-term solution for the mitigation of aircraft emissions. Use of RJF in commercial flights is already a reality, mostly after 2008 [5], although still on a modest scale. Recent examples include a series of 80 flights by KLM in Embraer E190 aircrafts from Oslo to Amsterdam employing *Camelina sativa*-based RJF produced by Neste through HEFA processing [6]. Unlike other biofuels, namely biodiesel and bioethanol, worldwide RJF utilization currently lacks incentive mechanisms [7], which are vital for the deployment of industrial units [8].

At present, Brazil is short of a clearly defined national policy to promote the use of RJF, despite recent movements concerning this possibility [9]. Brazil will be obliged to join the CORSIA instrument from 2027 onwards. Within its scope, it is estimated that around 1.5 million tonnes of CO₂ emissions will have to be avoided by 2030 to promote carbon-neutral expansion of international flights originating in the country alone. Besides, as a signatory of the Paris Agreement (COP-21), Brazil established an aggressive Nationally Determined Contribution (NDC) towards cutting GHG emissions. In the aviation sector, the carbon-neutral growth of the entire sector in the country starting in 2020 will require aviation to mitigate between 8.3 and 12.4 million tonnes of CO₂ emissions in 2030 [10]. Other nations, such as China, have also ratified challenging goals to reduce the carbon intensity of civil aviation up to 65% and peak emissions by 2030 [11]. Besides, the European Union has set shorter-term goals aiming at the displacement of 4% of fossil fuel consumption in 2020 – roughly equivalent to 2 million tonnes of RJF [12].

In order to tackle such ambitious goals, Brazil shows a prolific

panorama in terms of renewable energy production and biomass cultivation. One crop is specially cultivated for energy purposes: sugarcane, mostly converted into ethanol, sugar, and electricity. Ethanol distilleries can act as host plants for a series of integrated processes for biobased products, ranging from biodiesel [13] to bio-propylene [14], succinic acid [15], microalgal biomass [16], and advanced biofuels [17–19], among which RJF production is comprised. Sugarcane mills can supply electricity, process steam, and raw materials to integrated industrial conversion units, thus consisting in a good example of a true biorefinery concept. The main objective of establishing integrated biorefineries is to profit from process integration advantages to leverage one promising, incipient technological route with inputs of materials, energy, and other utilities coming from a consolidated, more robust plant. This is the case when using outputs from a sugarcane mill to supply an RJF production plant so that the latter can achieve better operational stability and economic performance, as well as lower environmental impacts. Although such biorefinery alternatives are not currently common in the country, their potential for RJF production should be evaluated so as to provide accurate and quantitative information to decision-making processes.

For the estimation of the potential of adding RJF production to the sugar-energy sector, techno-economic and environmental analyses of technological alternatives must be carried out. The work presented herein was developed by the Brazilian Bioethanol Science and Technology Laboratory (CTBE), in partnership with Embraer S.A. and The Boeing Company, concerning the possibility and feasibility of RJF (within SPK specification limits) production in the Brazilian context from different feedstocks in integrated biorefineries with ethanol distilleries. The Virtual Sugarcane Biorefinery (VSB), an innovative framework developed by CTBE [20], was employed in the sustainability assessment of different biorefinery alternatives. This study considered the establishment of completely self-sufficient biorefineries, i.e. which only take different types of biomass (sugarcane stalks and straw, eucalyptus, and vegetable oils) as main inputs and do not rely on external energy supply (e.g. electricity, natural gas, or other energy sources) for operation. Three production routes were analyzed, following their relevance in a worldwide context and their potential of large-scale deployment in Brazil: HEFA, FT, and ATJ [21]. In the designed scenarios, HEFA routes processed palm, macauba, or soybean oils, while FT conversion was based on gasification of either sugarcane lignocellulosic fractions or eucalyptus, and ATJ converted isobutanol or ethanol into RJF. All work was developed with data from both scientific and open literature, and with CTBE's know-how on Brazilian sugarcane biorefineries. The annual jet fuel output of each integrated biorefinery scenario is compared to a pre-determined jet fuel substitution target. In this work, RJF production was aimed at 5% of the conventional jet fuel consumption in Brazil in 2014¹ of 7.5 billion L [22], corresponding to the production of 375 million L of RJF/year.

When assessing techno-economic and environmental impacts of RJF production, authors often consider standalone plants, regardless of the feedstock: lipids (microalgae, *Pongamia pinnata*, *Jatropha curcas*, *Camelina sativa*, *Brassica carinata*, used cooking oil, and conventional vegetable oils) [23–30]; lignocellulosic material (LCM), such as poplar and sugarcane bagasse [31–34]; and alcohols [35]. The potential of RJF production in Brazil has been previously overviewed, also as independent plants [21,36]. The integration with sugarcane mills itself is an innovative configuration which mitigates risks inherent to RJF technologies. RJF production in integration with sugarcane mills has already been assessed for the ATJ technology in South Africa [35] and for both ATJ and SIP routes in Brazil [37]. Moreover, De Jong et al. [24] confirmed the advantages of integration between RJF production and (unspecified) incubator facilities to the reduction of minimum jet

¹ The following year saw a slight reduction of 1.5% in conventional jet fuel consumption, thus indicating the current stability of the Brazilian internal market.

fuel selling price (MJSP) between 4% and 8% in comparison to standalone RJF units. Nonetheless, the scientific literature lacks further efforts in assessing integrated biorefineries for other conversion routes. In this context, this study aims at comparing different strategies for RJF production integrated to sugarcane biorefineries in Brazil. The differentials of this analysis reside mainly in biorefinery simulation using rigorous models for the determination of complete mass and energy balances, as well as in the calculations integrating all steps of the production chain – from the agricultural phase to final fuel use. The biorefineries are ultimately assessed in terms of both economic and environmental performances and the produced RJF is benchmarked against conventional, fossil jet fuel by taking into account both economic and environmental aspects.

2. Materials and methods

2.1. Biorefinery configuration

2.1.1. Brazilian sugarcane mills

Sugarcane processing in Brazil occurs mainly with three different plant configurations: autonomous ethanol distillery (producing only ethanol from carbohydrates), sugar factory (producing only sugar), and sugar factory with an annexed ethanol distillery (producing both ethanol and sugar). Sugarcane bagasse and, occasionally, sugarcane straw are burned in Cogeneration of Heat and Power (CHP) units for the generation of process steam and electricity to supply the energetic requirements of the plant. When electricity production exceeds process demand, the surplus can be sold to the grid. In this study, optimized autonomous ethanol distilleries were chosen as host plants for the establishment of RJF-producing biorefineries. Both first-generation (1G) and integrated first- and second-generation (1G2G) distilleries were considered to supply inputs to RJF production. The base ethanol distillery refers to a modern plant with high-pressure boilers, reduced process steam consumption, and electric mill drivers. The distillery crushes four million tonnes of sugarcane/year and produces hydrous ethanol (93%, w/w) as the main product. The process uses 50% of the available sugarcane straw, recovered in bales in a second-pass straw harvesting operation, to expressively increase power output in comparison to mills which do not perform this operation. Process conditions and yields of second-generation (2G) ethanol production were mainly retrieved from medium-term technology estimates from Junqueira et al. [38]. General parameters of the distilleries can be found in publications using the VSB framework [20].

2.1.2. RJF route: HEFA

Most HEFA routes comprise the general steps shown in Fig. 1a or a

slight variation thereof. The assumed HEFA technology in this paper broadly follows the process proposed by Pearson [27], with an overall two-step hydrocarbon yield of around 80% from soybean oil. With this configuration, vegetable oil undergoes hydrogenation, propane loss, and deoxygenation in a hydrotreatment reactor for the removal of structural oxygen and carbon-carbon double bonds from triglycerides. Next, a hydrocracking reactor catalytically hydrogenates the reactional mixture from the first reactor to produce isomers and cracks long carbon chains into paraffinic, fuel-range molecules. For greater accuracy of mass and energy balances of each type of vegetable oil conversion, the reactions taking place in each reactor were accounted for in the determination of reaction heat and H_2 consumption. The final step involves fractionation of the products in two sequential atmospheric columns, the first separating off-gas and water with a second one distilling hydrocarbon fuels (green naphtha, RJF, and green diesel). Table 1 shows the main parameters of HEFA equipment employed in the simulations.

Three options of vegetable oils were assessed towards their potential of producing liquid hydrocarbons: palm, macauba, and soybean oils. Fatty acid profiles for each oil were retrieved from Tres et al. [49], Grossi [50], and Ndiaye et al. [51], respectively. The degree of unsaturation of fatty acids directly influences the amount of H_2 needed for the conversion of vegetable oils into liquid hydrocarbons. Table 1 summarizes the specific H_2 consumptions determined for each of the vegetable oils.

2.1.3. RJF route: FT

Fig. 1b shows a simplified process flow diagram of a generic biomass-based FT process for the production of liquid hydrocarbons. The amount of produced RJF is ultimately highly dependent on the process configuration, feedstock composition, and on the scale of the thermochemical plant [52]. In spite of RJF being the main product of interest in this assessment, FT routes were assumed to produce high quantities of green naphtha, following the design of coal-processing South African Fischer-Tropsch units [52]. The indirect gasifier and reformer system for biomass gasification were adapted from Dutta et al. [40], while cleaning of syngas was performed using the Rectisol® process and the FT synthesis itself was carried out using temperatures of around 200 °C [33]. Table 1 shows the main parameters of the route, while other general parameters of the thermochemical conversion of biomass can be found in Dias et al. [53] and in Morais et al. [54].

The biorefinery was designed to operate either with LCM from sugarcane, in the form of bagasse and straw, or eucalyptus. Eucalyptus has been historically used in Central-Western Brazil with an energetic focus, either as charcoal or in the form of logs. These biomasses have a similar composition in terms of carbon, hydrogen, and oxygen. Ultimate

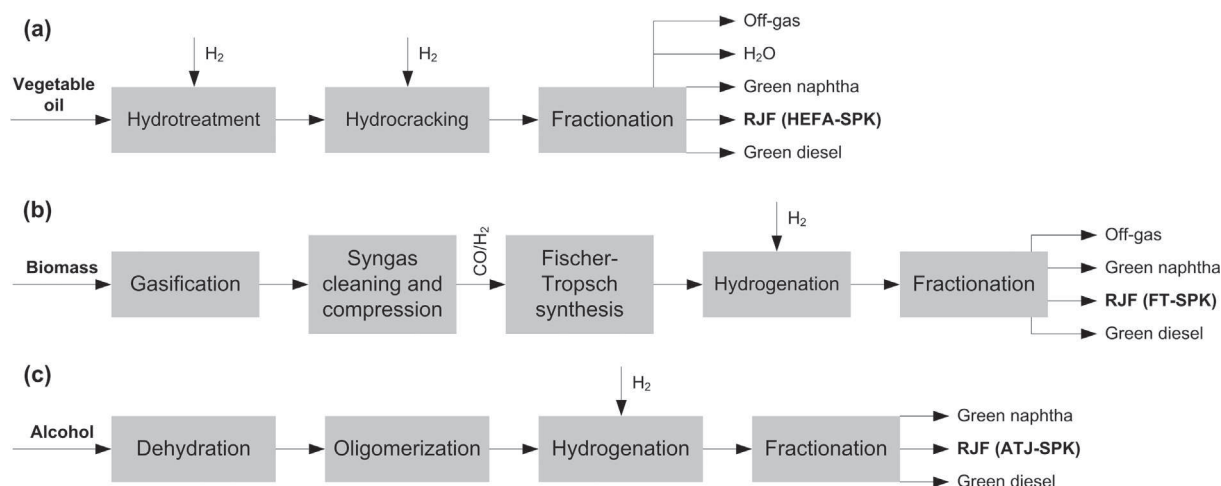


Fig. 1. Overall steps of RJF production via (a) Hydroprocessed Esters and Fatty Acids (HEFA), (b) Gasification and Fischer-Tropsch Synthesis (FT), and (c) Alcohol to Jet (ATJ) routes.

Table 1

Main technical parameters of the RJF production routes and auxiliary unit operations employed in the simulations.

Parameter	Value	Reference
HEFA		
Hydrotreatment reactor		
Temperature, pressure	325 °C, 34.5 bar	[27]
Hydrocracking reactor		
Temperature, pressure	280 °C, 55 bar	[39]
Overall hydrocarbon yield	0.8 kg/kg oil	[27]
Specific H ₂ consumption		
Palm oil	31.7 kg H ₂ /tonne oil	Calculated
Macauaba oil	33.3 kg H ₂ /tonne oil	Calculated
Soybean oil	37.7 kg H ₂ /tonne oil	Calculated
FT		
Gasifier		
Temperature	870 °C	[40]
Steam to biomass ratio	0.4 kg/kg biomass (d.b.)	[40]
Reformer		
Temperature	910 °C	[40]
Fischer-Tropsch synthesis		
Single-pass CO conversion to hydrocarbons	40%	[33]
ATJ		
Ethanol dehydration		
Temperature, pressure	450 °C, 11.4 bar	[41]
Ethanol conversion	99.5%	[41]
Ethylene oligomerization		
Temperature, pressure	120 °C, 35 bar	[42]
Ethylene conversion	99.3%	[42]
Isobutanol fermentation		
Fermentation time	21.5 h	[43,44]
Glucose conversion to isobutanol	0.288 g/g ^a	[43,44]
Isobutanol dehydration		
Temperature, pressure	310 °C, atmospheric	[45]
Isobutanol conversion	99.3%	[45]
Isobutylene oligomerization		
Temperature, pressure	160 °C, atmospheric	[44]
Isobutylene conversion	85%	[44]
Hydrogenation of oligomers		
Temperature, pressure	150 °C, 150 psi H ₂	[44]
Conversion	> 99%	[44]
Auxiliary unit operations		
Water electrolysis (WE)		
H ₂ yield	0.047 kg H ₂ /kg H ₂ O	[46]
Energy consumption	62.1 kWh/kg H ₂	[46]
Pressure swing adsorption (PSA)		
H ₂ recovery	93%	Consideration
Produced H ₂ purity	> 99%	Consideration
Internal combustion engine (ICE)		
Compression ratio	11:1	[47,48]

^a 70% yield of the maximum theoretical conversion of 0.411 g_{isobutanol}/g_{glucose}.

and proximate analyses of sugarcane and eucalyptus LCM were retrieved from the VSB database [53] and from Telmo et al. [55], respectively. It is imperative to note that the gasification process was considered to operate with coarse-ground biomass. This consideration is strong since the operation of a gasifier with such raw materials is not currently demonstrated in industrial scale, but achievable in the near-to-medium term. Additional costs for fine comminution of biomass or other pretreatment operations, such as fast pyrolysis for bio-oil production or torrefaction, would lead to an increase in both biomass [56] and RJF production costs. Consequently, the development of efficient pretreatment options is crucial for further development of this technology [57].

Apart from producing liquid hydrocarbons, thermochemical plants are known to generate significant amounts of energy. Thermal energy in the form of process steam is usually produced in heat recovery steam generators through the cooling of high-temperature process streams. Electricity, on the other hand, can be obtained in turboexpanders and in

dedicated gas turbines. The production of both process steam and electricity can also be modulated through diverting syngas from the synthesis step to combined cycle systems.

2.1.4. RJF route: ATJ

Fig. 1c depicts the conversion of alcohols to SPK with ATJ technology in four main steps. Green naphtha, green diesel, and RJF are the main products of the process. Two feedstocks for ATJ routes were assessed: ethanol (both 1G and 1G2G) and isobutanol. While ethanol is not a currently-approved feedstock for ATJ conversion, it was included in the analysis due to the obvious convenience of profiting from the large ethanol production in Brazil.

Process parameters for ethanol dehydration to ethylene and by-products were based on Arvidsson and Lundin [41]. Oligomerization and hydrogenation steps were simulated according to Heveling et al. [42] and Gruber et al. [44], respectively. The issuing liquid mixture is fractionated using conventional atmospheric distillation columns.

When considering isobutanol as the feedstock for ATJ-SPK production, the synthesis of the alcohol from sugarcane juice fermentation was considered to be similar to that of ethanol. Therefore, the steps prior to fermentation (e.g., sugar extraction and juice treatment) were assumed to be the same as those found in a conventional ethanol distillery. Process parameters for sugar fermentation to isobutanol were retrieved from Hawkins et al. [58]. Purification of isobutanol (up to 87.5%) was performed by azeotropic distillation since it forms a heterogeneous azeotrope with water. Isobutanol conversion to jet fuel, from dehydration to hydrogenation, was simulated according to examples available in Gruber et al. [44]. Table 1 presents the parameters considered for the simulation of ATJ routes.

2.1.5. Additional unit operations

Nearly every RJF production technology requires H₂ as a process input – namely SPK-producing ones. H₂ can be synthesized in a dedicated section through several possible techniques: biomass or fossil feedstock gasification, natural gas steam reforming, off-gas steam reforming, ethanol steam reforming, and water electrolysis (WE), among others [59–61]. In view of a self-sufficient biorefinery configuration adapted to the reality of Brazilian sugarcane mills, H₂ production was carried out through WE. Other H₂ production methods, such as methane steam reforming, were not considered due to two main reasons: avoiding the need of establishing the biorefineries close to the natural gas grid and maintaining a low dependence on fossil fuels. Positive sustainability impacts of WE, especially when coupled with renewable energy for operation, have already been demonstrated [62,63]. Besides, preliminary internal assessments showed that ethanol steam reforming for H₂ production is not an economically attractive option: despite having lower capital expenditure (CAPEX) than electrolyzers, the current poor H₂ yields [64] cause the technology to ultimately be an expensive alternative to such biorefineries. Besides, having ethanol as an output of the integrated plant is strategically important towards assuring the supply of liquid biofuels in Brazil. Therefore, WE was employed for H₂ production in HEFA and ATJ routes.

Pressure swing adsorption (PSA) units are required to ensure the separation and recycling of H₂ to reactors. In both HEFA and ATJ routes, H₂ is separated from the off-gas stream (containing propane, CO₂, and other light gases) for recycling. In the FT route, the PSA unit is responsible for the separation of H₂ from both clean and recycled syngas for subsequent hydrocarbon upgrading to liquid fuels. This equipment is considered to recover 93% of the H₂ contained in the input gas stream and produces H₂ with > 99% purity. Finally, process off-gas and PSA tail gas are either burned in fired heaters for thermal energy generation or in internal combustion engines (ICE) for additional electricity production, according to each case. Table 1 shows the main parameters of all employed auxiliary unit operations.

Table 2
Scenarios for the assessment of integrated biorefineries.

Scenario	RJF route	Main feedstock	Host ethanol distillery	H ₂ production method
HEFA1	HEFA	Palm oil	1G	Water electrolysis
HEFA2	HEFA	Macauba oil	1G	Water electrolysis
HEFA3	HEFA	Soybean oil	1G	Water electrolysis
FT1	FT	Sugarcane LCM	1G	Gasification
FT2	FT	Sugarcane and eucalyptus LCM	1G	Gasification
ATJ1	ATJ	Ethanol	1G	Water electrolysis
ATJ2	ATJ	Ethanol	1G2G	Water electrolysis
ATJ3	ATJ	Isobutanol	1G	Water electrolysis

2.2. Process simulation

Eight scenarios were designed, simulated, and evaluated, according to Table 2. Mass and energy balances of the integrated biorefineries were obtained from simulations using the Aspen Plus® process simulator version 8.6 (AspenTech, Bedford, MA, USA). Fig. 2 shows schematic flowsheets for each biorefinery scenario. All RJF biorefineries were benchmarked against a base ethanol distillery (BASE scenario) operating during sugarcane season, as described in Section 2.1.1.

The biorefineries were conceived to be self-sufficient in terms of energy, i.e., no external energy sources are needed apart from that generated with the required raw material inputs (sugarcane stalks and straw, vegetable oils, and eucalyptus, according to each case). RJF production benefits from the integration with ethanol distilleries through the utilization of energy vectors (process steam and electricity) and material outputs (sugarcane LCM, hydrous ethanol) issued from the

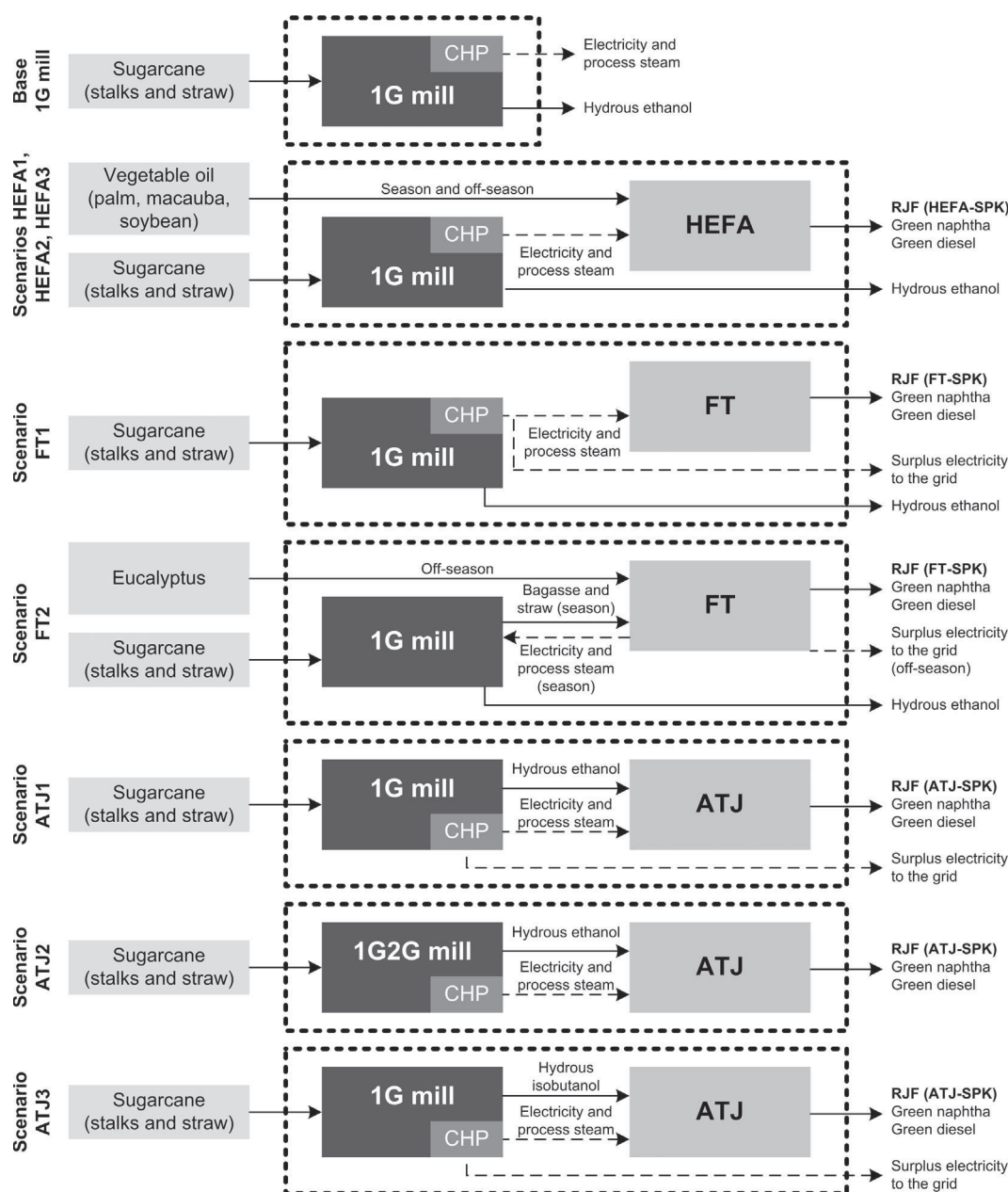


Fig. 2. Simplified flowsheet for each assessed biorefinery and associated scenarios.

mill. In FT biorefineries, the opposite may also happen: the sugarcane mill's energy requirements are supplied by the thermochemical plant.

Sugarcane mills crush sugarcane for ethanol production during sugarcane season (200 days/year). All RJF plants operate year-round (330 days/year) with constant feedstock input: vegetable oil for HEFA, sugarcane and eucalyptus LCM for FT, and alcohols for ATJ. CHP units of sugarcane mills are the only sections to operate year-round in order to supply steam and electricity to the RJF production plant.

For the design of the integrated biorefineries, some practical limits were set for the determination of the size of the annexed RJF facility. HEFA plant capacity is limited by the available surplus electricity from the sugarcane mill for H₂ production (scenarios HEFA1, HEFA2, and HEFA3). The capacity of each FT unit is determined by the amount of processed biomass. In scenario FT1, part of the sugarcane LCM (bagasse and straw) is stored during season for off-season operation of the annexed FT plant. Scenario FT2, on the other hand, processes all sugarcane LCM during season and an equal hourly flow of eucalyptus LCM during off-season. Since considerations for scenario FT1 give origin to a relatively low-scale thermochemical plant, the supply of the total amount of energy required by the sugarcane mill during season is complemented by a small CHP unit consuming about a third of the total available sugarcane LCM. The thermochemical plant in scenario FT2 is of larger capacity, as well as its energy generation capability; therefore, no CHP unit in the ethanol distillery is required. Finally, in all ATJ scenarios, the RJF plant capacities were defined to consume all alcohol (ethanol or isobutanol) produced in the sugarcane mill. In these biorefineries, part of the produced ethanol is stored for operation of the ATJ process in the off-season.

2.3. Techno-economic assessment

2.3.1. Biomass production

The CanaSoft model of the VSB framework [65] was employed to determine production costs of the different biomasses considered in the assessment. The economic inventories were calculated based on the main parameters for each biomass production system (e.g. yield, agricultural operations and type of used machinery, fertilizer application rates, among others). These calculations are linked to databases containing comprehensive information about all agricultural operations used in biomass production and transportation systems, including agricultural performance parameters for different types of harvesters, tractors, and implements, as well as their weight, costs, diesel consumption, annual use, lifespan, and depreciation [65]. Originally modeled to describe sugarcane production processes, the CanaSoft model has already been adapted to assess other biomasses such as energy cane, corn, soybean, and sunn hemp [20,38,66,67]. In this study, the agricultural production systems of macauba, palm, and eucalyptus were also included in the model using the same approach. The sugarcane production system in a typical Brazilian mill was based on Dias et al. [53] and Cavalett et al. [65]. The soybean production system was considered to follow the production process described by Agrianual [68] and Silva et al. [69], with typical parameters for a highly technified system in Central-Western Brazil. Technical parameters from Agrianual [70] and Macêdo et al. [71] were used to describe the palm oil production system. For macauba cultivation, since there is no commercial production system, the palm production system was used as a reference, with important adaptations using data from the literature [72,73] and consultation with experts in the field (personal communication with Colombo C, Azevedo Filho JA, and Siqueira WJ. Instituto Agrônomo de Campinas (IAC), Brazil, December 2015 and February 2016). Finally, the characterization of the production system of commercial forests in Brazil was based on literature data [68,74–77].

The minimum selling prices (MSP) of vegetable oils were determined by considering the revenues of all coproducts obtained from the processing of palm and macauba fruits and soybean grains in extraction plants. The calculated figure is the price of vegetable oil that

would lead the extraction plant to an Internal Rate of Return (IRR) of 12% (minimum acceptable rate of return or MARR). Capital cost remuneration of the plant is also included in the analysis. Transport costs for vegetable oil delivery at the biorefinery were also included for final oil cost estimation. Fig. 3 shows the locations of extraction plants for each feedstock and for the sugarcane biorefinery. Transport distances for palm, macauba, and soybean oils were estimated at 2000 km, 500 km, and 250 km, respectively. Palm and macauba crops mainly yield fresh fruit bunches (including fruits, stalks, and stems), while soybean crops produce grains. Soybean grain processing generates soybean meal (which is responsible for nearly 70% of the plant's revenues), soybean oil, and lecithin. Electricity for the plant's operation is bought from the grid and process steam is generated with natural gas. In the case of palm and macauba processing, the process is self-sufficient in terms of energy through the burning of stalks and stems of fresh fruit bunches. Besides the vegetable oil, palm processing also generates palm kernel oil, palm kernel meal, and surplus electricity. Macauba processing, on the other hand, produces macauba oil, macauba kernel oil, and macauba kernel meal. Prices of palm kernel and macauba kernel meal were estimated according to their protein contents with soybean meal as the reference. Protein contents of soybean, palm kernel, and macauba kernel meals are 44%, 35%, and 14.5%, respectively.

It was assumed that eucalyptus logs are produced, harvested, and transported to the biorefinery of scenario FT2 in a radius of 250 km from the sugarcane mill.

Agricultural operations and transport of sugarcane stalks and straw consume around 4 L of diesel/tonne of sugarcane, according to internal VSB estimates. Since a fuel fraction equivalent to diesel is obtained in every assessed scenario and the agricultural production of sugarcane is verticalized with the industrial plant, the produced green diesel was considered to replace fossil diesel in such operations. This practice helps both reducing the overall biomass production cost and lowering associated environmental impacts [53]. In this way, green diesel for sugarcane production is acquired from the industrial unit by paying the taxes that would normally be included in diesel by a distributor (e.g. PIS/COFINS of US\$ 0.064/L and ICMS of 15% for the Brazilian state of Goiás, amounting to US\$ 0.067/L).

2.3.2. Biorefinery economic performance

Several steps comprise the economic assessment of the selected scenarios. After simulation of each process and dimensioning of related equipment, CAPEX was estimated for each biorefinery module, mainly the ethanol distillery and the many components of the RJF plant: main processing equipment, H₂ production, PSA unit, and additional equipment for energy production. CAPEX of ethanol distilleries were determined using the internal database of the VSB, created through partnerships with engineering companies from the sugar-energy sector. In scenario ATJ3, the CAPEX of the distillery was estimated by substituting the ethanol fermentation and distillation sections by isobutanol-producing ones. Estimates for the main equipment of HEFA, FT, and ATJ technologies were retrieved from the scientific literature [27,40,78,79]. Capital costs of H₂ production via water electrolysis were fetched from Langås [80]. For CAPEX estimation purposes, a location factor of 1.4 was considered for imported systems, specifically the gasification section of FT plants and WE equipment for H₂ production in HEFA and ATJ plants. Other equipment of HEFA, ATJ, and the remainder of FT plants, as well as energy generation machinery and PSA units, were assumed to be available in Brazil in the medium-term. CAPEX of ICEs in HEFA scenarios and in scenario ATJ2 were calculated at 770 € per installed kW (personal communication with equipment manufacturers). Whenever needed, exchanges rates of 3.86 and 4.23 were used for conversion from US\$ and € to R\$, respectively (average rates as of December/2015). It is relevant to point out that these values are among the highest ones in the recent economic history of Brazil.

Hydrocarbon selling prices were calculated based on historical

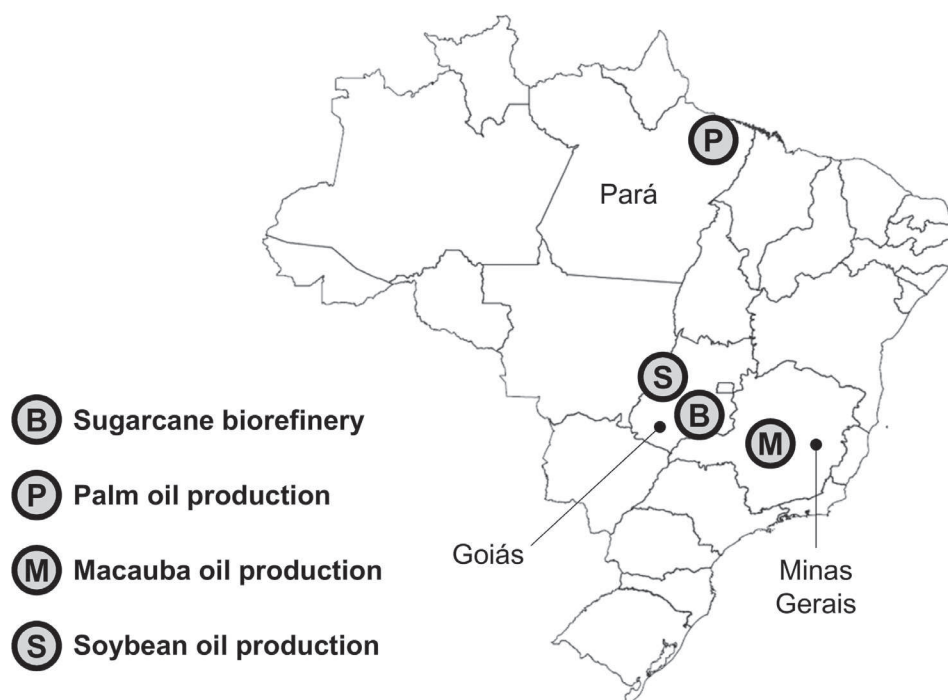


Fig. 3. Considered locations for vegetable oil extraction plants and ethanol distilleries in Brazil.

Table 3

Considered selling prices for biorefinery products based on Brazilian historical market data.

Product	Value	Unit
Hydrous ethanol	0.35	US\$/L
Naphtha (green naphtha)	0.54	US\$/L
Jet fuel (RJF)	0.50	US\$/L
Diesel (green diesel)	0.45	US\$/L
Electricity	47.27	US\$/MWh

market data retrieved from the National Agency of Petroleum, Natural Gas, and Biofuels (ANP). Prices were updated to December/2015 using the Brazilian inflation rate and refer to products delivered at the factory gate (without taxes). Since long-term jet fuel and diesel historical price series are available, a 6-year moving average was employed in a 10-year price series for selling price estimation. For naphtha, a simple average was used in a 3-year historical price series for adjusted price determination due to a lack of further data in Brazil. Hydrous ethanol selling price was also calculated based on a 6-year moving average of data retrieved from a 10-year historical series provided by the Center for Advanced Studies on Applied Economics (CEPEA). Finally, electricity selling price was obtained from a 10-year historical average of energy auctions in Brazil, considering only biomass-generated energy. Table 3 compiles the resulting product prices used in the analysis.

Operational expenses (OPEX) include costs with biomass (sugarcane stalks and straws in all scenarios, vegetable oils in scenarios HEFA1, HEFA2, and HEFA3, and eucalyptus in scenario FT2), costs with inputs for 1G ethanol production (chemicals for sugarcane juice treatment, for example) and 2G ethanol production (enzymes and yeasts), costs with plant maintenance and labor, and costs with RJF production (reactor catalysts, gasification bed material, PSA unit adsorbent, and other industrial consumables).

The development of a discounted cash flow for each greenfield biorefinery depended on other important economic considerations: working capital of 10% of the CAPEX; maintenance cost corresponding to 3% of the CAPEX; biorefinery lifespan of 25 years; annual depreciation of 10%; and income tax of 34% [81]. The economic performance of each scenario was assessed in terms of two main economic

indices retrieved from the discounted cash flow methodology, namely IRR and MJSP. The MJSP is calculated analogously to the MSP of vegetable oils: the selling price of RJF is varied until the IRR of the biorefinery attains a MARR of 12%. Further information on the used methodology and data can be found in Watanabe et al. [81].

2.4. Environmental assessment

Life Cycle Assessment methodology (LCA) was used for the quantitative assessment of environmental impacts. This method is described in the ISO 14000 series of standards [82,83] and is the most used worldwide methodology for the environmental assessment of products and processes, including bioenergy production systems [84–88]. The LCA technique considers impacts in emissions and in the use of resources typically included in the most common environmental assessments of bioenergy systems. Substantially broader environmental aspects can be covered with LCA approach, ranging from climate change and fossil resource depletion to acidification, toxicity, and land use aspects.

The SimaPro software [89] was used as a supporting tool and the ecoinvent database v2.2 [90] was employed to obtain the environmental profile of background product systems (e.g. diesel, fertilizers, pesticides, and other chemicals used as inputs in the processes). In the LCA methodology, the use of resources and emissions to soil, air, and water of the entire production chain are converted into different environmental impact categories using internationally-recognized environmental impact assessment methods. In this context, selected impacts categories from ReCipe Midpoint method [91] were used to compare the environmental performances of the assessed scenarios.

The climate change impact category (also called “carbon footprint”, “global warming potential” or “GHG emissions”) is measured in g CO₂ eq. The characterization factor describing the radiative forcing of one mass-based unit of a given greenhouse gas relative to that of CO₂ over a time frame of 100 years is obtained from the 2007 Intergovernmental Panel on Climate Change (IPCC) method [92]. This method has global consensus on the relationship between GHG and the increase in global temperature.

The human toxicity impact category concerns effects of toxic substances on the human environment. The characterization factors

Table 4
Main inputs and outputs of the integrated biorefineries and associated agricultural results.

RJF route	BASE	HEFA		FT		ATJ	
Scenario	1G	HEFA1	HEFA2	HEFA3	FT1	FT2	ATJ1
RJF feedstock	–	Palm oil	Macauba oil	Soybean oil	Sugarcane	Sugarcane + Eucalyptus	1G EtOH
							1G2G EtOH
							ATJ3
							Isobutanol
Inputs							
Sugarcane (million tonnes/y)	4.00	4.00	4.00	4.00	4.00	4.00	4.00
Straw (million tonnes/y)	0.18	0.18	0.18	0.18	0.18	0.18	0.18
Eucalyptus (million tonnes/y)	–	–	–	–	–	–	–
Vegetable oil (million tonnes/y)	–	0.40	0.39	0.34	–	–	–
Outputs							
Total green diesel production (million L/y)	–	122	118	105	33	81	11
Green diesel sold to market (million L/y)	–	105	101	87	16	64	0
RJF (million L/y)	–	267	258	228	42	102	140
Green naphtha (million L/y)	–	35	34	30	53	129	58
Hydrous ethanol (million L/y)	360	360	360	360	360	360	0
Electricity (GWh/y)	769	0	0	0	156	45	0
Agricultural parameters							
Sugarcane area per biorefinery (ha)	52,632	52,632	52,632	52,632	52,632	52,632	52,632
Eucalyptus area per biorefinery (ha)	–	–	–	–	–	–	–
Oil crop area per biorefinery (ha)	–	121,554	72,166	613,569	–	–	–
Number of biorefineries to 5% target	–	2	2	2	9	4	3
Total area to 5% target (ha)	–	348,371	249,595	1,332,400	473,684	341,270	157,895

account for the environmental persistence (fate) and accumulation in the human food chain (exposure), and toxicity (effect) of a chemical [93].

The category named terrestrial acidification reflects the atmospheric deposition of inorganic substances, such as sulfates, nitrates, and phosphates, which cause a change in soil acidity [94]. The geographical scale varies from local to continental.

The agricultural land occupation impact category can be defined as the maintenance of an area in a particular state over a particular time period. It reflects the damage to ecosystems due to the effects of the occupation of land for agricultural production [91].

The fossil depletion category considers the gradual decrease of quantity and quality of fossil resources. Since fossil resources become depleted and more costly, other resources need to be exploited. The characterization factors are based on the projected change in the supply mix between conventional and unconventional oil sources [91].

Life cycle inventories used in this assessment were obtained from agricultural and industrial simulations of mass and energy balances. Since multiple products are obtained in each plant, it is necessary to split part of the environmental impacts to each one of them. In this study, an allocation procedure based on economic relationships was chosen, as detailed in Watanabe et al. [81]. Boundaries of the system include the stages of agricultural production, transport of biomass to industrial units, transportation of oil between extraction and sugarcane biorefineries (for HEFA routes), industrial conversion, transport of RJF to airports, and use in aircraft turbines considering typical emissions of international flights.

3. Results and discussion

3.1. Technical results

Table 4 summarizes the main inputs and outputs of the assessed scenarios. The BASE scenario produces 360 million L of ethanol/year and a considerable amount of surplus electricity to the grid (769 MWh/year). This number is significantly higher than that found in the average Brazilian sugarcane mill, with a non-optimized operation, process inefficiencies, and without straw recovery. In all integrated biorefineries, as detailed in Section 2.3.1, the produced green diesel is used to partially or totally substitute the 17 million L/year of fossil diesel consumed during agricultural operations and transport of sugarcane stalks and straw recovery. Table 4 presents both the total output of green diesel by the industrial unit and the quantity sold to the market, after fossil diesel substitution. HEFA and FT biorefineries achieve 100% fossil fuel substitution since these units can easily produce more green diesel than the required amount. Green diesel output in all ATJ scenarios is lower than the needed 17 million L/year, therefore resulting in fossil diesel substitution of 51%, 67%, and 22% in scenarios ATJ1, ATJ2, and ATJ3, respectively. The output of liquid hydrocarbons by a given biorefinery is highly dependent on the consumption of additional biomass: processing eucalyptus or vegetable oils besides sugarcane naturally increases the total production of liquid hydrocarbons of a scenario in comparison with a biorefinery that relies exclusively on sugarcane biomass to operate. Specific production of hydrocarbons in HEFA biorefineries were calculated at between 0.94 and 0.98 L of hydrocarbons/L of vegetable oil, while FT processing yielded 0.16 and 0.23 L of hydrocarbons/kg of LCM (dry basis) for scenarios FT1 and FT2, respectively, and ATJ processing produced 0.47 L of hydrocarbons/L of hydrous ethanol (93%, w/w) and 0.68 L of hydrocarbons/L of hydrous isobutanol (87.5%, w/w). These figures can widely vary according to different process configurations within each technology, especially in FT scenarios, in which LCM is employed for electricity generation besides the synthesis of liquid hydrocarbons. The main inputs of RJF facilities are detailed in Supplementary Data 1.

RJF production is also highly variable among scenarios. The highest outputs can be found in HEFA scenarios, while the lowest ones were

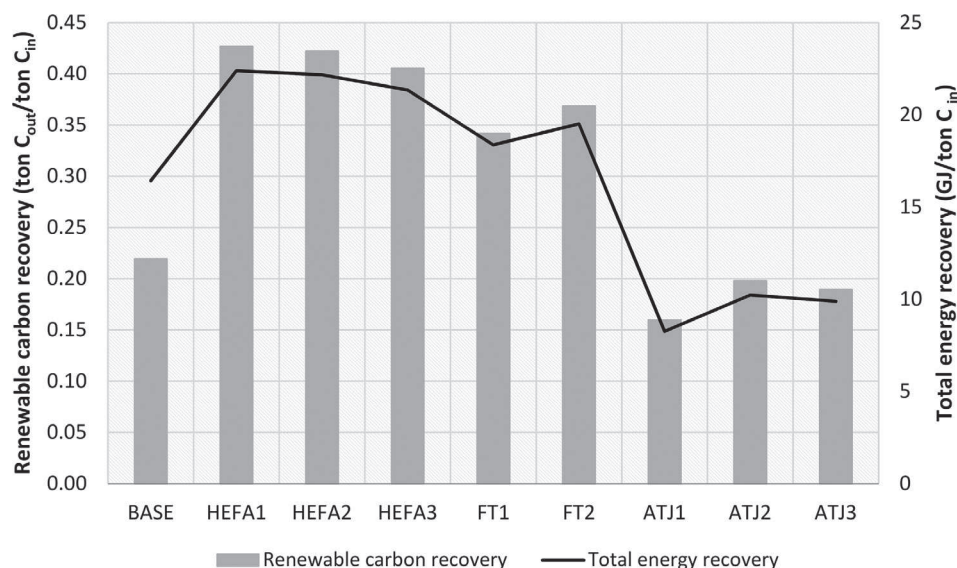


Fig. 4. Comparison of biorefining efficiency among assessed scenarios in terms of renewable carbon recovery in liquid biofuels and total energy recovery per renewable carbon input. Solid bars represent the amount of renewable carbon recovered as liquid biofuels, while the solid line indicates the total retrieved energy, including liquid biofuels and electricity.

obtained in scenarios FT1, FT2, and ATJ1. A single integrated biorefinery can supply between 11% (scenario FT1) and 71% (scenario HEFA1) of the predefined 5% fossil jet fuel substitution target. Inversely, the amount of needed facilities to reach the same objective drops from nine plants mirroring scenario FT1 to only two facilities in the case of HEFA biorefineries. Table 4 also shows results related to the direct occupation of agricultural land, thus allowing to glimpse the proportions involved in the production of RJF in a Brazilian context. In scenarios ATJ2 and ATJ3, three identical biorefineries consuming only sugarcane require nearly 158 thousand hectares of agricultural land to slightly surpass the 5% conventional jet fuel substitution target. On the other end, soybean oil processing in two biorefineries of scenario HEFA3 would demand more than 1.3 million hectares – equivalent to 4% of the 33 million ha cultivated with soybean nowadays [95]. Macauba and palm HEFA biorefineries (scenarios HEFA1 and HEFA2) produce larger amounts of RJF than their soybean counterpart and require much less area: around 250 thousand hectares for macauba and 350 thousand hectares for palm. It is important to reiterate that the establishment of two identical biorefineries, as the ones from scenario HEFA1 or HEFA2, is enough to reach and surpass the target of 5% fossil jet fuel substitution.

The amount of H₂ needed for hydrocarbon upgrading in each biorefinery alternative is highly variable. HEFA plants require nearly 2000 kg of H₂/h, which is in the same order of magnitude of the consumption by conventional oil refineries. Decentralized electricity production is also an important feature of the biorefineries: in scenarios HEFA1, HEFA2, and HEFA3, ICEs are responsible for the generation of additional 31 MW, 30 MW, and 26 MW, respectively, through the combustion of PSA tail gas. Since the extra energy is mainly used in further H₂ synthesis, this strategy ultimately improves the vegetable oil processing capacity of biorefineries.

Fig. 4 shows estimates towards the biorefining efficiency of the integrated plants. Two indices were determined to rank the assessed plants in terms of their ability in converting biomass into usable energy: renewable carbon recovery and total energy recovery. The indicators are normalized by the total renewable carbon input in the biorefinery in the form of sugarcane (stalks, vegetable impurities, and straw), vegetable oils, and eucalyptus. Due to the consumption of extra biomass, all HEFA scenarios and scenario FT2 display total renewable carbon input of over 895 thousand tonnes/year. All other scenarios are limited to the 636 thousand tonnes of carbon/year provided by sugarcane fractions alone. In view of the high hydrocarbon yield of RJF production via HEFA routes [27], such biorefineries are the most efficient ones for the conversion of different types of biomass, with over 0.40 tonnes of

Table 5

Production costs of sugarcane stalks and straw with green diesel use in agricultural operations.

Sugarcane fraction	Scenario			
	HEFA and FT	ATJ1	ATJ2	ATJ3
Stalks (US\$/tonne)	16.49	17.18	16.96	17.58
Straw (US\$/tonne ^a)	17.74	19.02	18.61	19.76
Fossil diesel substitution by green diesel	100%	51%	67%	22%

^a Dry basis.

Table 6

Price composition of palm, macauba, and soybean oils.

Vegetable oil	Palm	Macauba	Soybean
Feedstock cost ^a (US\$/tonne)	65 ^b	51 ^b	193 ^c
Vegetable oil MSP ^a (US\$/tonne)	344	316	420
Delivered oil price ^d (US\$/tonne)	409	333	430

^a At extraction plant gate.

^b Cost per tonne of fresh fruit bunches.

^c Cost per tonne of fresh grains.

^d At RJF plant gate.

carbon recovered per tonne of carbon input. FT technologies have a similarly high efficiency, with carbon recovery attaining 0.37 tonnes per tonne of consumed carbon. Finally, ATJ biorefineries present efficiencies even lower than conventional 1G ethanol distilleries. This is a natural outcome considering that the RJF production plant consumes two finished products from the sugarcane mill, i.e. hydrous ethanol and electricity, for the synthesis of hydrocarbons.

3.2. Economic results

Due to the verticalization of the production chain envisaged for the scenarios, the use of green diesel in agricultural operations reduces the production costs of both sugarcane stalks and straw. When fossil diesel is used, the calculated production costs of sugarcane stalks and straw (dry basis) are US\$ 17.89/tonne and US\$ 20.33/tonne, respectively. The removal of intermediaries in the diesel supply chain, as well as transportation costs, significantly affects the final cost of green diesel for sugarcane cultivation, harvesting, and transportation, thus consisting in a real competitive advantage for this type of biorefinery. As a

Table 7
CAPEX and main economic results of the assessed scenarios.

RJF route	BASE	HEFA			FT		ATJ		
Scenario	1G	HEFA1	HEFA2	HEFA3	FT1	FT2	ATJ1	ATJ2	ATJ3
RJF feedstock	–	Palm oil	Macauba oil	Soybean oil	Sugarcane	Sugarcane + Eucalyptus	1G EtOH	1G2G EtOH	Isobutanol
Detailed CAPEX (US\$ million)									
Ethanol distillery	224	194	194	194	131	104	194	298	220
Annexed SPK technology									
Main equipment	–	222	217	201	213	414	60	72	67
H ₂ production	–	88	87	85	–	–	20	26	16
PSA unit	–	24	22	19	–	–	–	–	–
Additional energy production	–	26	25	22	2	–	–	14	–
TOTAL CAPEX (US\$ million)	–	553	545	520	347	519	274	410	303
Economic performance									
IRR (%)	19.3%	3.7%	9.2%	3.6%	16.5%	13.5%	0.6%	NC ^a	5.7%
MJSP (US\$/L)	–	0.66	0.55	0.71	–0.22	0.36	0.87	1.17	0.68

^a Non-calculated IRR. Revenues in scenario ATJ2 from sales are lower than the associated operational expenses.

matter of comparison, Table 5 shows the production costs of sugarcane stalks and straw for all scenarios with green diesel use.

Table 6 depicts the main results for vegetable oil MSP. Eucalyptus are delivered to the biorefinery of scenario FT2 at a cost of US\$ 39.07/m³ of logs (roughly US\$ 95.28/tonne of logs).

Table 7 shows detailed CAPEX estimates for the base 1G sugarcane mill (BASE) and the assessed biorefineries, divided into CAPEX for the ethanol distillery and for the annexed SPK production technology. All HEFA scenarios and scenario ATJ1 are integrated to ethanol distilleries with the same configuration, with a CAPEX of US\$ 194 million. In scenario FT2, the FT route is integrated to an ethanol distillery with no CHP unit and, therefore, with a lower CAPEX (US\$ 104 million), while the ethanol distillery of scenario FT1 presents a CAPEX of US\$ 131 million due to the need for a small CHP unit. Scenario ATJ2 involves the use of a 1G2G ethanol distillery, a plant with considerably higher capital investment in view of the equipment employed in sugarcane LCM processing into 2G ethanol. For comparison, the BASE scenario presents a CAPEX of US\$ 224 million as a result of higher investments in the CHP section, since all available LCM is processed during the sugarcane harvest season.

CAPEX estimates for the annexed RJF routes are divided into four categories: main equipment for liquid hydrocarbons synthesis, H₂ production section, PSA unit for H₂ recovery, and additional energy production. In HEFA scenarios, the required H₂ flow reaches up to 2000 kg/h. Production of H₂ was set as 15% higher than the determined specific consumption to compensate losses due to the separation efficiency of PSA units. Thus, the H₂ production section was designed as two parallel electrolysis modules because of the considerable size of the equipment. Electrolyzers demanding nearly 50 MW of power are not currently produced in Brazil and their acquisition passes through importing from foreign producers. In ATJ scenarios, single electrolyzers were considered for CAPEX estimates due to the smaller size required in comparison to those needed for HEFA processing. CAPEX for PSA units in HEFA biorefineries were also discriminated considering the large size of the equipment involved. In this analysis, excess H₂ must be separated and recycled to the reactors for the process to be both technically and economically feasible because the operation is carried out with a stoichiometric excess of H₂. Finally, additional equipment for energy production is needed in some biorefineries, such as ICEs in HEFA biorefineries and in scenario ATJ2 burning off-gases and green naphtha, respectively.

Table 7 also presents the determined IRRs. The base 1G sugarcane mill presents a higher IRR (19.3%) than the integrated biorefineries in view of the intrinsic simplicity of the employed unit operations and maturity of the ethanol production process after 40 years of

development in Brazil. Among HEFA technologies, macauba oil processing into liquid hydrocarbons (scenario HEFA2) yields the best economic results (although lower than the MARR). Vegetable oil prices play an important role in defining the economic performance of HEFA biorefineries. Since macauba oil is cheaper than either palm oil or soybean oil when delivered at the biorefinery gate, the calculated IRR is expected to be the highest. Still, cost with vegetable oil amounts to 73%, 68%, and 70% of the total cost in scenarios HEFA1, HEFA2, and HEFA3, respectively. The best biorefineries in terms of economic results were the FT scenarios, both with IRR higher than the MARR. Despite the advantages brought to CAPEX of scenario FT2 by an economy of scale of the thermochemical plant, the IRR is lower than that of scenario FT1 due to a significantly higher cost of biomass for off-season operation (eucalyptus logs in comparison to sugarcane LCM). It is also important to highlight that the overall economic results of FT biorefineries are highly influenced by the revenue of hydrous ethanol commercialization, which represent 66% and 46% of the total revenue in scenarios FT1 and FT2, respectively. Both scenarios benefit from a distillery with lower CAPEX as the result of a small CHP unit (scenario FT1) or its absence (scenario FT2) for the reduction of the total fixed capital cost. In this way, it can be said that the FT thermochemical route greatly profits from the integration with ethanol distilleries, with superior economic indices than standalone FT plants [32,35]. However, when considering the deployment of the technology on existing sugarcane mills, the FT route is among the most difficult ones to be established. This occurs as a consequence of the high requirement of mass and energy integration between processes, something not easily done in a brownfield biorefinery considering the necessity of redesigning the utility section of the host distillery. HEFA and ATJ technologies, on the other hand, are more dependent on modular equipment and their integration to existing sugarcane mills is inherently simpler. Finally, employing ATJ technology in sugarcane biorefineries did not present satisfactory economic results. Production of ATJ-SPK via isobutanol presented the largest IRR, although still lower than the MARR. The main reason for the weak economic performance is the overall yield of the process. ATJ technologies convert inputs with a considerable market price (hydrous ethanol and hydrous isobutanol) into hydrocarbons with low profit margin and with low yield.

Fig. 5 presents MJSP results for each integrated biorefinery. FT scenarios yielded the best results (of R\$ –0.22/L and R\$ 0.36/L), since the selling of hydrous ethanol and green naphtha is responsible for most of the revenues of such biorefineries; therefore, the burden on the selling price of RJF is lower than in the other evaluated plants. In other words, the commercialization of the remaining coproducts of the biorefinery could account alone for an IRR of 12% or higher, thus a

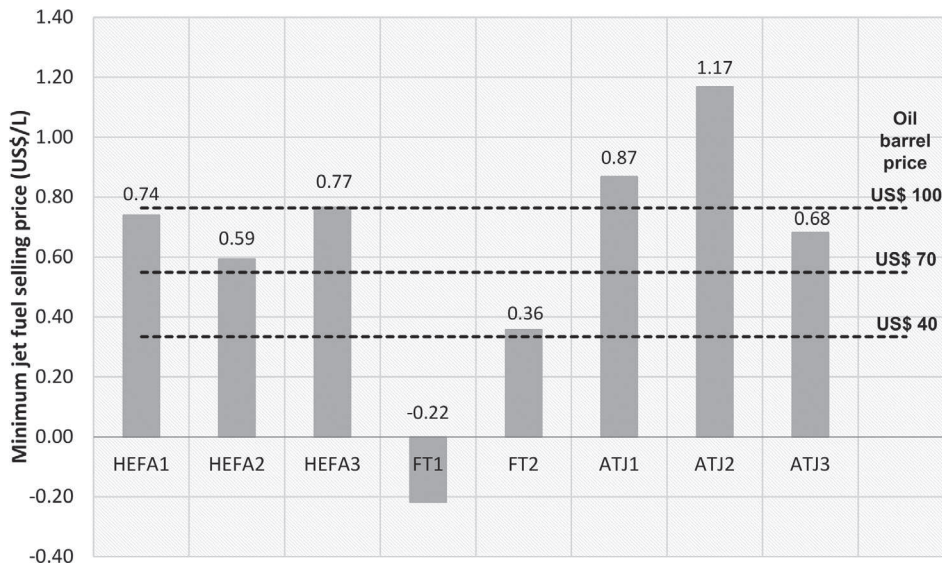


Fig. 5. Calculated minimum jet fuel selling price (MJSP) and comparison with the equivalent fossil jet fuel price as a function of the oil barrel price.

negative MJSP in scenario FT1. Pereira et al. [28] also determined that the commercialization of coproducts is fundamental towards the economic feasibility of RJF production. Fig. 5 also provides a comparison between MJSP and conventional jet fuel selling prices according to the international crude oil price. For this analysis, data was retrieved from the U.S. Energy Information Administration [96]. In the United States,

jet fuel selling price is highly dependent on crude oil price, the former being positively correlated with the latter. The oil barrel price used in the analysis corresponds to the Europe Brent spot price, free on board (FOB). An ocean freight rate of US\$ 37/tonne of jet fuel (in clean tankers) was considered to transport the fuel from the U.S. Gulf Coast to the Port of Santos (state of São Paulo, Brazil). In this way, the calculated

Table 8
Typical RJF production costs and MSP found in the literature.

Conversion route	Feedstock	Economic result			Reference
		Value	Index	Base year	
HDO	<i>Camelina sativa</i> <i>Brassica carinata</i> Used cooking oil	0.69 US\$/L 0.74 US\$/L 0.74 US\$/L	Break-even cost Break-even cost Break-even cost	2015	[23]
HEFA	Used cooking oil	1.31 €/kg	MSP, 10% discount rate	2014	[24]
FT	Forest residues	1.69 €/kg			
	Wheat straw	2.44 €/kg			
HTL	Forest residues	0.95 €/kg			
	Wheat straw	1.33 €/kg			
HDCJ	Forest residues	1.35 €/kg			
	Wheat straw	1.82 €/kg			
ATJ	Forest residues	2.31 €/kg			
	Wheat straw	3.41 €/kg			
DSHC	Forest residues	4.60 €/kg			
	Wheat straw	6.18 €/kg			
HVO	Microalgae	1,343 US\$/BOE	MSP, 10% discount rate	2011	[25]
	<i>Pongamia pinnata</i>	374 US\$/BOE			
	Sugarcane molasses	301 US\$/BOE			
FT	Woody biomass	1.24 €/L	MSP, 10% discount rate	Unspecified	[31]
ATJ (mixed alcohols from syngas, modified FT catalyst)	Woody biomass	1.49 €/L			
ATJ (mixed alcohols from syngas, modified methanol catalyst)	Woody biomass	1.28 €/L			
ATJ (via ethyl acetate and ethanol)	Poplar LCM	1.14–1.79 US\$/L	MSP, 15% discount rate	2014	[32]
		0.67–0.86 US\$/L	Cash cost		
HDO (after aldol condensation of furfural and levulinic acid)	Corn cob	1.05–1.45 US\$/L	MSP, 10% discount rate	Unspecified	[34]
ATJ (via 2G ethanol)	LCM	3.43 US\$/kg	MSP, 10% discount rate	2014	[35]
ATJ (via gasification and syngas fermentation to ethanol)	LCM	2.49 US\$/kg			
FT	LCM	2.44 US\$/kg			
HEFA	Vegetable oil (unspecified)	2.22 US\$/kg			
ATJ (via 1G ethanol)	Sugarcane sucrose	2.54 US\$/kg			

BOE: barrel of oil equivalent.

DSHC: Direct Fermentation of Sugars to Hydrocarbons (equivalent to SIP).

HDCJ: Hydrotreated Depolymerized Cellulosic Jet.

HDO: Hydrodeoxygenation.

HTL: Hydrothermal Liquefaction.

HVO: Hydrotreated Vegetable Oil (equivalent to HEFA).

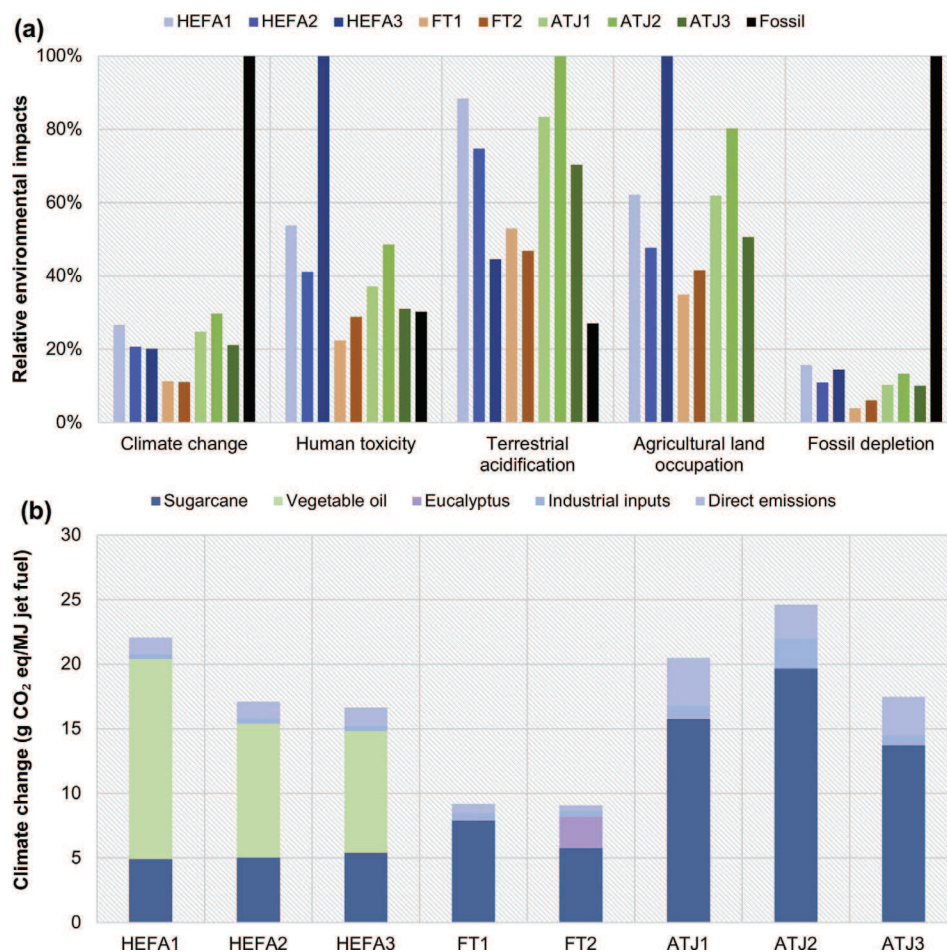


Fig. 6. Environmental impacts of renewable jet fuel (RJV) production: (a) assessed impact categories and (b) breakdown of GHG emissions.

conventional jet fuel selling prices associated with US\$ 40, US\$ 70, and US\$ 100 oil barrels are of US\$ 0.33/L, US\$ 0.55/L, and US\$ 0.76/L, respectively. This analysis can indicate which technologies and scenarios can competitively produce RJF according to the international oil barrel price. For instance, with the 2016 level of US\$ 40 oil barrel, only scenario FT1 presents MJSP lower than the associated US\$ 0.33/L conventional jet fuel selling price.

The determined economic results can be compared to those obtained in the scientific literature (summarized in Table 8). The wide variability of feedstocks and conversion routes considered by different authors gives rise to an equally diverse spectrum of economic results, ranging from as low as US\$ 0.67/L for an ATJ route using poplar LCM as feedstock [32] up to € 6.18/kg (about US\$ 5.42/L) for the direct fermentation of sugars from wheat straw [24]. It is interesting to note that many factors impact this type of analysis, such as plant scale, type of RJF produced, the country considered in the assessment, and economic parameters (mainly discount rate and methodology). In average, the figures determined in this work remain in agreement with the literature, especially for HEFA and ATJ routes. The FT technology highly benefits from the integration with sugarcane mills and from sales of coproducts of the biorefinery to significantly lower the associated MJSP.

3.3. Environmental results

Fig. 6a shows the comparative life cycle environmental results of the assessed scenarios. All the stages of the life cycle are covered in the results, from raw material extraction from nature, biomass production and conversion into products, transportation systems, and final jet fuel use in aircraft engines (considering average emissions of

intercontinental flights). Fossil jet fuel is also included in this assessment as a baseline for comparison.

It is possible to see that RJF produced in integrated sugarcane biorefineries always presents better environmental results for global scale impact categories (climate change and fossil depletion) when compared to the fossil alternative. On the other hand, biofuels present higher impacts for local environmental impacts categories (human toxicity, terrestrial acidification, and agricultural land occupation), mainly due to the intrinsic impacts of the agricultural stages of the production chain.

Among RJF production routes, in general, FT scenarios achieved the best environmental performance. Scenario FT1 does not require other biomass resources than sugarcane, therefore not adding extra impacts related to the agricultural phase. In scenario FT2, impacts of eucalyptus production are almost entirely compensated by the increased production of hydrocarbons during sugarcane off-season period. In climate change and terrestrial acidification categories, in fact, scenario FT2 presented slightly lower impacts, since these categories are strongly dependent on fertilizers used in agricultural stage and eucalyptus crops require fewer inputs than sugarcane.

The main reason for the relatively poor environmental performance of ATJ scenarios is the overall conversion yield. When ethanol or isobutanol are converted into RJF, fewer coproducts are available to allocate the overall environmental impacts. The large amount of inputs required to produce vegetable oils also led HEFA scenarios to present the highest environmental impacts. Fertilizers and diesel used in palm, macauba, and soybean cultivation, as well as diesel used in the transportation of vegetable oil to the biorefineries, are responsible for the higher impacts in fossil depletion in these scenarios. Agrochemicals used in oil-based plants cultivation highly contribute to the results

Table 9
Requirements for GHG mitigation in Brazil by 2030 following the CORSIA mechanism and the NDC.

RJF route	BASE		HEFA		FT		ATJ		ATJ3	
Scenario	IG	HEFA1	HEFA2	HEFA3	FT1	FT2	ATJ1	ATJ2	ATJ3	Isobutanol
RJF feedstock	–	Palm oil	Macabua oil	Soybean oil	Sugarcane	Sugarcane + Eucalyptus	1G EtOH	1G2G EtOH	1G2G EtOH	Isobutanol
Climate change impacts (g CO₂ eq/MJ jet fuel)	–	22.3	17.3	16.9	9.4	9.3	20.7	24.8	17.7	
Reduction in climate change impacts^a (g CO₂ eq/MJ jet fuel)	–	61.3	66.3	66.7	74.2	74.3	62.9	58.8	65.9	
CORSIA										
Needed RJF production (million L/y)	–	765	707	702	632	631	748	801	706	
Number of biorefineries	–	3	3	4	7	16	8	6	5	
Total agricultural area (ha)	–	522,558	374,394	2,664,804	368,424	1,365,088	421,056	315,792	263,160	
Total investment (US\$ billion)	–	1.7	1.6	2.1	3.6	5.6	2.2	2.5	1.5	
NDC (low target)										
Needed RJF production (million L/y)	–	4,230	3,912	3,885	3,495	3,491	4,141	4,432	3,905	
Number of biorefineries	–	16	16	18	35	84	39	32	25	
Total agricultural area (ha)	–	2,786,976	1,996,768	11,991,618	1,842,120	7,166,712	2,052,648	1,684,224	1,315,800	
Total investment (US\$ billion)	–	8.8	8.7	9.4	18.2	29.1	10.7	13.1	7.6	
NDC (high target)										
Needed RJF production (million L/y)	–	6,320	5,845	5,804	5,222	5,215	6,187	6,621	5,834	
Number of biorefineries	–	24	23	26	52	125	59	48	37	
Total agricultural area (ha)	–	4,180,464	2,870,354	17,321,226	2,736,864	10,664,750	3,105,288	2,526,336	1,947,384	
Total investment (US\$ billion)	–	13.3	12.5	13.5	27.0	43.4	16.1	19.7	11.2	

^a In comparison to fossil jet fuel (climate change impacts of 83.6 g CO₂ eq/MJ jet fuel).

observed in HEFA biorefineries, especially in the soybean-based one. This scenario is also affected by low per-hectare soybean yields compared to palm and macabua, leading to greater impacts on agricultural land occupation.

Despite the great differences between scenarios, all of them showed a reduction of over 70% in GHG emissions compared to the fossil baseline, hence being classified as advanced biofuels according to regulations of the Renewable Fuel Standard of the United States Environmental Protection Agency [97]. Concerning RJF production via ethanol dehydration, in a similar route to scenarios ATJ1 and ATJ2, Budberg et al. [98] determined GHG emissions ranging between 32 and 73 g CO₂ eq/MJ jet fuel. The environmental performance of the route is highly dependent on the H₂ production method: steam reforming of natural gas, for example, would yield higher impacts than gasification of LCM. In this way, employing water electrolysis greatly benefits the overall impacts of RJF production, with a maximum value of 25 g CO₂ eq/MJ jet fuel determined for scenario ATJ2. De Jong et al. [99] reached a similar conclusion, in which the use of sustainable energy sources for H₂ production helps in reducing GHG emissions of RJF. When analyzing analogous routes, Trivedi et al. [100] also pointed out the need of employing renewable energy for H₂ synthesis as a means of producing RJF with lower dependence on fossil sources.

Fig. 6b depicts the breakdown of climate change impacts for the assessed RJF scenarios at the production stage (not including the impacts of use phase). It is possible to see that the impact is concentrated in the biomass production phase of both sugarcane and vegetable oils, mainly due to fertilizers and diesel use – these impacts are particularly higher in ATJ scenarios since fossil diesel is still required.

3.4. Contribution towards mitigation of GHG emissions in Brazil

For Brazil to meet the GHG mitigation targets proposed in both CORSIA and NDC mechanisms, a wide array of RJF production plants will have to be established in the country. Table 9 presents the magnitude of this task with regards to the amount of required RJF, as well as the number of biorefineries needed to produce it, the dedicated agricultural area for biomass production, and the total investment involved in establishing the industrial units. Taking the CORSIA instrument alone, between 630 and 800 million L of RJF/year in 2030 will be needed to ensure the carbon-neutral growth of international flights originating in Brazil. This amount could be met with three to 16 biorefineries matching those of the assessed scenarios. When considering the NDC targets, which are significantly larger than those determined for the CORSIA mechanism, the lowest level of GHG mitigation (8.3 million tonnes of CO₂) would require between 3.5 and 4.4 billion L of RJF/year by 2030 produced by tens of industrial units and at a total investment of at least US\$ 7.5 billion. The panorama is even more severe taking into account the highest projections of GHG mitigation (12.4 million tonnes of CO₂). For example, if soybean oil was to be the only feedstock for RJF synthesis, the total agricultural area for the grain would increase over 50%, from 33 million ha to more than 50 million ha. It is worthwhile mentioning that the establishment of such biorefineries entails the production of electricity and several other liquid biofuels as coproducts, which ultimately contributes towards the overall energy security of Brazil. These figures allow policymakers to perceive the urgent need for a National Program in order to address the issue.

4. Conclusions

The present study assessed the potential of producing RJF in integrated biorefineries with ethanol distilleries in Brazil. The variability of the obtained results shows that the mitigation of GHG emissions in the country is highly dependent on the feedstock, RJF production route, and plant location. FT scenarios had the best economic results: IRR of the integrated biorefineries and MJSP. HEFA biorefineries presented

the largest volumes of RJF production due to the processing of vegetable oil with high efficiency. Finally, all biorefineries produced RJF with low climate change impacts – at least 70% reduction in comparison to fossil jet fuel.

The best option for supplying RJF in Brazil passes through the optimization of certain parameters and assumptions. This includes the refinement of process simulations for the most promising scenarios with data on RJF production provided by the industry. Other developments comprise the determination of the best possible biorefinery locations depending on the conversion technology and locally available feedstocks. Additionally, solving the RJF supply issue in Brazil in the future may also pass through combining several biorefinery alternatives into the matrix – and not from one exclusive route. For example, macauba-based RJF production could be carried out in Minas Gerais, while São Paulo state could rely on FT routes and Southern Brazil on soybean and other feedstocks.

In this way, the innovation towards the assessment of RJF routes is clear in this study, since results of integrated sugarcane-RJF biorefineries are not common in the scientific literature and those presented herein enable the discussion of RJF production at scientific, economic, environmental, and policymaking levels.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.apenergy.2017.10.079>.

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