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Techno-economic and greenhouse gas emissions assessment

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Integrated 1st and 2nd generation sugarcane bio-refinery for jet fuel production in Brazil: Techno-economic and greenhouse gas emissions assessment

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This study presents a techno-economic analysis and an environmental assessment, of the whole production chain (biomass production, sugar extraction, biomass pretreatment, sugars fermentation, and products recovery and purification), of a fully autarkic sugarcane-based biorefinery for biojet fuel production. All scenarios considered correspond to *1st/2nd* generation integrated biorefineries (*i.e.* simultaneous use of sugarcane juice stream and lignocellulosic fractions) with a production scale of 208 kton (biojet fuel) yr^{-1}. In this paper, we compared multiple options for the most relevant processing steps of the biorefinery: eight biomass pretreatment technologies (*i.e.* dilute acid, dilute acid + alkaline treatment, steam explosion, steam explosion + alkaline treatment, organosolv, alkaline wet oxidation, liquid hot water and liquid hot water + alkaline treatment); two biojet fuel production routes from sugars (*i.e.* ethanol to jet and direct fermentation); one biojet fuel production route from biomass (*i.e.* fast pyrolysis); two biojet fuel production routes from lignin obtained after biomass pretreatment (*i.e.* fast pyrolysis and gasification Fischer- Tropsch); and one alternative use for lignin (*i.e.* co-generation). From the combination of these key features, 81 scenarios are selected and compared. Furthermore, three potential technological improvements were analysed for selected scenarios: *i)* recovery of acetic acid and furfural (for cases with bagasse pretreatment); *ii*) production of succinic acid from a fraction of concentrated juice; *iii)* increase of operation time (from 200 to 320 days yr^{-1}) by using sweet sorghum as cumulative feedstock. The different scenarios are compared first based on the minimum jet fuel selling price (MJSP) and then based on their environmental performance (*i.e.* greenhouse gas (GHG) emissions and non-renewable energy use (NREU)). Among the scenarios considering biomass pretreatment, the lower MJSP are obtained when 1G/2G sugars are upgraded via ethanol fermentation (ETJ) (*i.e.* SO_2 steam explosion: 3409 US $.ton^{-1}, and wet oxidation: 3230 US $.ton^{-1}). Additional technological improvements may help to further reduce the MJSP either marginally (2%, by using 1G sugars for succinic acid production) or significantly (30%, by increasing the operation time). Thus, the lowest MJSP here calculated is 1725 US $.ton^{-1} (with 1G sugars to biojet fuel via ethanol, and bagasse to biojet fuel via fast pyrolysis). Finally, for all scenarios considered, the GHG emissions and NREU were found to be lower than 42.5 kg CO_2eq.GJ^{-1} and 700 MJ GJ^{-1} respectively (except for scenarios with fast pyrolysis of bagasse where those figures were further reduced by 50% and 80% respectively). Although, the MJSP calculated for all scenarios are higher than those of the fossil jet fuel reference, the significant potential for environmental impacts reduction (in terms of GHG emissions and primary energy use) are encouraging for further research in costs reduction and technology development.

1. Introduction

The share in global anthropogenic greenhouse gas emissions (GHG) from the aviation sector will raise above the present 2–3%

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[1] as a consequence of passenger numbers duplication from 2016 to 2035 [2]. Thus, aviation companies are actively supporting projects that develop a sustainable and economically competitive crude oil jet fuel substitute. The target is to neutralize carbon emissions by 2030 and to reduce them in 50% by 2050. The alternative jet fuel must be "drop-in" like, allowing blending with crude oil jet with no technical changes to aircrafts [3].

Brazil will establish itself as the third largest domestic flights market and it is also a country with a long trajectory on the biofuels sector (*i.e.* bioethanol) supported by a mature sugarcane (SC) industry [4]. These combination of advantageous conditions, from both the feedstock supply side and the jet fuel demand end, puts Brazil in a highly potentially competitive situation for early development and implementation of biojet fuel production at commercial scale. Therefore, this paper explores the technical possibilities to align the well-established sugarcane industry with the new market opportunities within the Brazilian growing aviation sector given the sector's commitment to reduce its overall carbon footprint.

Recently, a few techno-economic studies have been published comparing alternative technologies and/or feedstocks for renewable jet fuel (RJF) production [5–8]. However, those studies focus solely on the RJF production technologies (both ASTM approved or soon to be approved). In this paper, we broaden the scope of the research to cover the complete supply chain considering Brazil as case-study; it includes: logistic aspects (*i.e.* transportation costs depending on specific locations for feedstock fields, mills, biorefinery facilities and airports to be supplied) and valorisation of all input streams (from a cradle-to-gate + combustion approach) to enhance economic performance (*i.e.* lower the minimum jet selling price (MJSP)) and reduce environmental impacts (greenhouse gas (GHG) emissions and non-renewable energy use (NREU)).

The MJSP determined in this project are comparatively more realistic for four main reasons: *i)* consideration of maximal capacity of technologies and auxiliary sections (*i.e.* wastewater treatment, H_2 steam methane reforming, and co-generation units); *ii)* use of geographical and temporal specific factors for prices of equipment and raw materials; *iii)* coverage of the entire supply chain for mass balances, utilities requirements, and mass/heat integration; and *iv)* detailed Aspen simulation, equipment design and heat/water integration for selected scenarios. Thus, in this paper we perform a techno-economic analysis of an autarkic greenfield biojet refinery in Brazil, in which the feedstock - sugarcane - is simultaneously used in *1st* and *2nd* generation integrated processes. The best scenarios are selected considering economic competitiveness, technological and logistics feasibility and environmental sustainability.

2. Methods and data collection

This section describes first the most important stages of the biorefinery supply chains, their battery limits and related technological details (incl. data used and sources), and then presents the methods used for techno-economic analysis and environmental assessment. The detailed description of technologies and related data are largely based on literature reporting operating conditions of specific processing units and their performance in terms of key parameters (*e.g.* selectivities, yields, efficiencies, among others). Given the large variability of processing conditions and performance indicators reported literature, all collected technical data were analysed (before use) to assess their source reliability, consistency through literature and suitability for a harmonized comparison of technologies. The selected technical data are used to model the biorefinery systems which in turn provide the inputs (*e.g.* equipment size, material flows, utilities requirements) for the economic analysis and environmental assessment models. Thus, quality and comparability of data and results were always checked.

2.1. Supply chain and logistics

The aim of the project was to cover 10% of jet fuel demand of Guarulhos (São Paulo) and Galeão (Rio de Janeiro) airports in the short term, *i.e.* 2020. Considering that a 50% blend with fossil jet fuel is acceptable, independently of the technology considered [9,10], the production capacity would be 208.9 kton biojet yr^{-1} [11–13].

Two fractions of sugarcane were considered: stalk, containing juice and bagasse; and straw, containing tops and leaves. The former is transported to mills and further processed while the latter (about 140 kg ton^{-1} SC) is considered to be partially left in the fields and up to 82 kg ton^{-1} SC can be used in the biorefinery co-generation section [14].

SC based biorefineries are limited by the seasonality of its harvesting period to 200 days yr^{-1}, however this period can be extended up to 320 days yr^{-1} considering that sweet sorghum (SS) is a plant with many physicochemical similarities to SC and that its harvesting season is between two cane cycles [15,16]. The detailed composition of stalks and bagasse after milling, field productivity and harvesting season for both feedstocks is summarized in Section A of the Supporting Information (SI).

Since sugarcane and extracted juice are susceptible to contamination, their storability is limited to less than 48 h, and therefore mills and biorefineries must be located nearby the sugarcane fields [13,17]. Thus, Campinas was the location selected for SC mills and biorefineries due to the high density of sugarcane mills in the area of São Paulo state and its proximity to the Guarulhos airport. To reduce logistics related costs, each mill was coupled with a biorefinery (pretreatment, fermentation, thermochemical upgrade) and both installations were integrated with auxiliary sections. Jet fuel is then transported 150 km to Guarulhos airport (São Paulo) and 570 km to Galeão airport (Rio de Janeiro). SC plantation in Brazil follows a ratooning practice (sugarcane regrows from shoots of previous cycles, up to 6 years), hence it was assumed that SS fields were located around SC fields [18]. As a consequence, SC is transported for 10 km, which is the radius occupied by a sugarcane field with a daily productivity of 12000 ton day^{-1} (maximum SC milling capacity) and SS is transported for 22 km.

2.2. System boundaries and scenarios definition

Fig. 1 depicts the processing sections included in the techno-economic analysis and environmental assessment. In the latter, feedstock growth and harvesting activities were considered, while in the former such activities were assumed to be already included in the feedstock price.

Reference scenarios are defined by two major features: *i)* use of 1G sugars (*i.e.* full use for biojet fuel production or partially sold for valorisation into value-added products, succinic acid in this case); and *ii*) use of bagasse (*i.e.* direct conversion into biojet fuel via fast pyrolysis (FP) or pretreatment for 2G sugars recovery). Furthermore, for biojet fuel production from 1G sugars two alternative technologies are considered, *i.e.* direct fermentation (DF) via farnesene and ethanol to jetfuel (ETJ). In the case of bagasse pretreatment for 2G sugars recovery, eight technologies are assessed (*i.e.* dilute acid (DA), dilute acid + alkaline treatment (DA-A), steam explosion (SE), steam explosion + alkaline treatment (SE-A), organosolv (O), wet oxidation (WO), liquid hot water (LHW) and liquid hot water + alkaline treatment (LHW-A)). Furthermore, among the scenarios considering bagasse pretreatment, an extra

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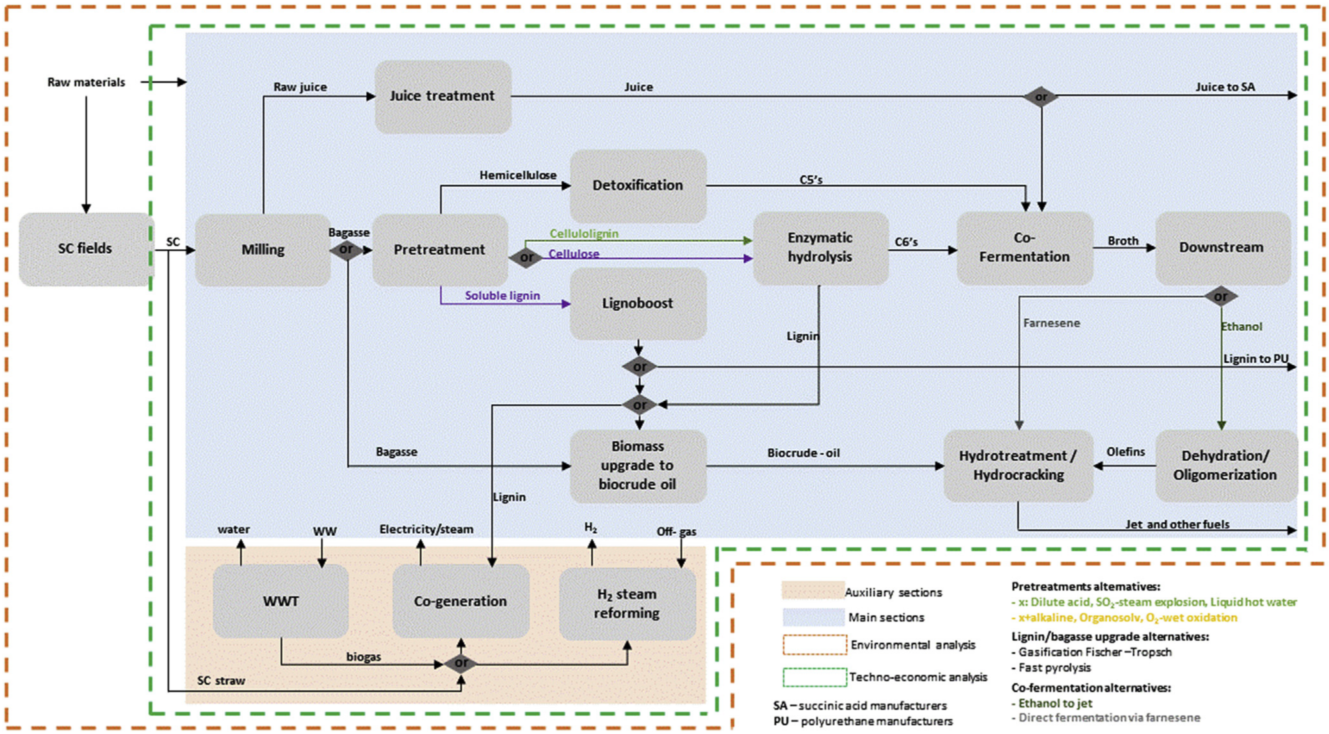

Fig. 1. Schematic representation of processing sections, and system boundaries for the techno-economic analysis and the environmental assessment.

section for recovery of acetic acid and furfural is considered as an additional technological possibility to improve the economic performance of the overall biorefinery. After pretreatment, the resulting streams undergo to detoxification and enzymatic hydrolysis prior to fermentation as shown in Fig. 1. In case of the lignin fraction, four possibilities are considered, *i.e.* co-generation, biojet fuel production via fast pyrolysis (FPJ), biojet fuel production via gasification Fischer–Tropsch (GFT), or selling a high purity lignin stream to polyurethane (PU) manufacturers.

Auxiliary sections (*i.e.* wastewater treatment (WWT), H_2 steam methane reforming (H_2 SMR) and co-generation) are specifically designed for each scenario since the wastewater streams, flue gas flow, process water, H_2 production, electricity consumption, steam requirements, solid waste streams, lignin production and non-hydrolysed biomass flow are different for each scenario.

In all cases, transportation costs of feedstocks, SC trash, sugarcane juice and biojet fuel, as well as the selling prices of the energy and material co-products were included in the economic analysis. To do so, the products specifications and the used prices are listed Sections B and C of the SI.

2.3. Technologies description and processing conditions

2.3.1. Milling

Milling includes SC cleaning and crushing, raw juice liming, settling, filtration and concentration of juice in multi-effect evaporators [19,20] with consumption of H_3PO_4, CaO, flocculant polymer and water, respectively, of 0.2, 1, 0.0025, 1.18 kg ton^{-1} SC. Then, 95% [19,20] and 92% [21] of sugars in the juice of SC and SS are recovered, respectively. Juice is then concentrated up to 65 wt.% when sold for external production of SA. For ETJ and DFJ fermentations the maximal product concentration allowed (EtOH and farnesene) are $\leq$10 wt.% [22] and 12.4 wt.% [23] respectively. Furthermore, the concentration of the fermentation and cellulase inhibitors must remain below limiting concentration, *i.e.* soluble lignin and acetic acid $\leq$5 g L^{-1} [24], and furans (furfural and 5-HMF) $\leq$ 0.3 g L^{-1} [25–27].

2.3.2. Bagasse pretreatment technologies

Several technologies have been reported in literature for bagasse pretreatment. The text below describes key aspects of the most relevant technologies while Section D.1. of the SI compares their technical advantages/disadvantages, operational conditions and CAPEX/OPEX (capital and operation expenses), including also the detoxification methods. Yields of pretreatment and enzymatic hydrolysis of each pretreatment considered are summarized in Table 1.

Diluted acid (DA), steam explosion (SE) and **liquid hot water (LHW)** produce two streams after pretreatment: hemicellulose hydrolysate and cellulolignin. The former undergoes detoxification while the latter is washed and re-filtered and both are then sent to enzymatic hydrolysis, after pH correction to 5 [28]. The difference is the catalyst used, respectively, H_2SO_4, SO_2 and biomass hydrolysed acetic acid [29], and on the solids loading. When **alkaline (A)** pretreatment is added, cellulolignin is fractionated in two streams: cellulose and black liquor. The latter contains solubilized lignin that is then precipitated via lignoboost process [30]. Lignoboost hydrolysate stream is then detoxified, along with hemicellulose hydrolysate. In the **Organosolv (O)** coupled with acid catalysis, solubilisation of lignin is guaranteed by the addition of acetone to the pretreatment [31] which, however, increases capital and operational costs due the addition of distillation for solvent recovery (99.5% assumed) [32]. **Wet oxidation (WO)** with Na_2CO_3 also allows lignin solubilisation but required extra capital investment due to an air separation unit (ASU) for O_2 production where a post-hydrolysis step is required [32]. Both O and WO include lignin precipitation via lignoboost [30]. The cases of WO and LHW are here designed and simulated in detail due to the lack of

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Table 1
Summary of process conditions and yields of pretreatments and enzymatic hydrolysis.

Parameter	DA [28]	SE [35]	O[k,l] [32,36]	WO[n,o,t] [37]	WO detail[u,v,w,x,z] [38,39]	LHW[q,r] [29]	LHW detail[y,z] [29]	A[s,t] [35]
Pretreatment[a,b]								
P (bar)/T °C/RT (min)	190/11/15	13/190/15	15/175/60	13/195/25	12/185	12/200/15	13.7/195	100/11/60
Solid loading (%)	20 [40]	30 [41]	20	20[p]	20	12	12	10 [40]
Catalyst/concentration (%)	H_2SO_4/1.5	SO_2/1.1	H_2SO_4/1.25[m]	Na_2CO_3/3[m] O_2/0.011[m]	Na_2CO_3/3[m] O_2[u]/0.003		CH_3COOH of hydrolysis/1.63	NaOH/1
Hydrolysis yields (%)								
Cellulose[c]	13.1	9.8	9.5	7.9	7.9	12	12	17
Hemicellulose[d]	90.8	82.6	79.1	93.0	93.0	84	84	72.5
Lignin[e]	4.7	13	85 [42]	51.5	51.5	5 [43]	5 [43]	91.0
Sugars dehydration Xylose[f]/Glucose[g] [41]	5.0	5.0	5.0	5.9/0	5.9/0	8.0/0	8.0/0	–
Deacetylation[h]	100	100	100	100	100	100	100	–
pH correction salt/concentration (g/L^{-1})[i]	NH_4OH/25	NaOH/5.4	NH_4OH/6.9	NH_4OH/4.4	–	–	NH_4OH/25.7	–
Enzymatic hydrolysis yields (%)[j]								
Cellulose	70 [20]	75 [44]	90 [32]	80 [37]	75	70 [45]	65	+20% [46]
Hemicellulose	65	65	70	70	65	70	65	+5%

[a] Continuous operation mode, solid/liquid filtrations with 100% efficiency, washing water/filter inlet of 0.3, or 0.47 [32] when cellulolignin is recovered, or 0.125 [30] when lignoboost lignin is recovered, were assumed in all pretreatments.
[b] In hemicellulose detoxification, the three multi-effects was assumed to evaporate 63% water, 39% of acetic acid and 77% of furfural from the inlet and to precipitate 60% of the soluble lignin [32]. Binding efficiencies of GAC (adsorbed compound/inlet compound) considered were: soluble lignin, furans, organic acids (assumed undissociated as pH is below their pKa) sugars/sugar oligomers, respectively, 88, 94, 24, 4% [47].
[c] $cellulose + 0.111\ H_2O \rightarrow 1.111\ glucose$.
[d] $xylan + 0.136\ H_2O \rightarrow 1.136\ xylose$ unless stated, this also represents arabinan hydrolysis.
[e] $lignin \rightarrow soluble\ lignin$.
[f] $xylose \rightarrow 0.64\ furfural + 0.36 H_2O$.
[g] $glucose \rightarrow 0.75 - HMF + 0.3 H_2O$.
[h] $acetate + H^+ \rightarrow acetic\ acid$. Stoichiometry from Ref. [40].
[i] Flowrate estimated based on stream composition.
[j] Enzyme loading was - 0.042 g cellulase g^{-1}cellulose [20], 0.044 g β-glucosidase g^{-1} dry biomass [20], 0.006 g xylanase g^{-1} cellulose [48].
[k] Acetone/water - 60/40 [42] and two GAC columns in series were used for hemicellulose detoxification.
[l] Organosolv also solubilized 99.7% of the ash [41].
[m] 1.25% is the proportion of H_2SO_4 catalyst compared with bagasse inlet.
[n] In WO, cellulose and hemicellulose hydrolysis yields led to glucose and C5 oligomers, respectively. Sugar oligomers hydrolysis occurred with these yields: glucose oligomer – 30.0%; xylose oligomer – 14.4%; arabinose oligomer – 67.0% [37].
[o] Post-hydrolysis: 5 bar, 135 °C, 60 min [32], hydrolysis of sugar oligomers to single sugars yield – 100%.
[p] [49] had 30%, but [37] had 6%, so 20% was assumed.
[q] *Laser* et al. [29], recommends 8%, but *Tao* et al. [50], considers 15%, so the average was assumed.
[r] In LHW, cellulose and hemicellulose hydrolysis yields led to glucose and C5 oligomers, respectively. Sugar oligomers hydrolysis occurred with these yields: glucose oligomer – 13.0%; xylose oligomer – 14.5%; arabinose oligomer – 14.5% [51]. This partial hydrolysis justifies the lower enzymatic hydrolysis yields in LHW.
[s] Alkaline pretreatment solubilized 69.9% of the ash [35].
[t] Lignoboost process required 0.048 ton CO_2 ton^{-1} of black liquor. Procedure described in Ref. [30], with a lignin recovery of 90% [52] with 28% moisture [30].
[u] O_2 pressure in the reactor bottom was 13 bar (estimated for a bubble column with 20 × 4 m). O_2 reacted was 5.13% of the O_2 inlet, estimated considering COD (chemical oxygen demand) variation from inlet/outlet in *Martin* et al., [37]. In the detailed WO, 100% of non-reacted O_2 was recovered in the ASU (air separation unit) and recycled to the process.
[v] Lignoboost simulated in Aspen Plus included precipitation with 0.25 kg CO_2 kg^{-1} lignin and 0.2 kg H_2SO_4 kg^{-1} lignin following the procedure in Ref. [53]. 80% of the soluble lignin, entering lignoboost was recovered with a moisture of 7%.
[w] Post-hydrolysis similar to WO one, but sugar oligomers hydrolysis yield was reduced to 92.8%.
[x] Acetic acid (AA) and furfural (FF) recovery occurred via L/L extraction with MTBE (100% recycled) and distillation. 25% of AA was recovered with ≈80% purity and 12% of FF was recovered with 99.5% purity.
[y] 12% of AA was recovered with ≈80% purity and 16% of FF was recovered with 99.5% purity.
[z] Enthalpies of pretreatment reaction considered in Aspen Plus simulation were: cellulose, xylan, arabinan, oligomers – 172.2 MJ mol^{-1} [54]; xylose, glucose, acetate - –138.6 MJ mol^{-1} [55]; lignin - 24.34 MJ mol^{-1} [56]. Reference T, P, state were, respectively, 25 °C, 1 atm and liquid.

scientific literature to compare against the other pretreatment alternatives. For detailed design and simulation of WO and LHW, the reaction yields from Table 1 are kept, but the equipment recovery yields are more conservative. Water and energy use are optimized and an acetic acid and furfural recovery section is also included. In WO, hemicellulose detoxification is also included. Detailed process conditions of both pretreatments are resumed in Section E.1 of SI.

Granulated activated carbon (GAC) adsorption is selected as the **hemicellulose detoxification** due to its reduced CAPEX and high removal efficiencies, except for organic acids [33]. To tackle this problem, a multi-effect evaporator is added to pretreatments before the GAC column (see Table 1).

As part of the detailed simulation, **enzymatic hydrolysis** was considered to be 5% less efficient due to high concentration of lignin from LHW and WO (2.5 g L^{-1} and 5 g L^{-1}, respectively) [34].

2.3.3. Fermentation and intermediate products upgrade to biojet

Two major fermentative pathways are considered for RJF manufacturing: alcohol to jet (ATJ) and direct fermentation via farnesene (DFJ) [6] (see Table 2). In ETJ, C5 and C6 sugars are fermented to ethanol, which is then recovered via distillation. Next, ethanol is dehydrated to ethylene, then condensed to butylene [57] and later oligomerized [10]. Hydrogenation [5] and distillation [19] allow the recovery of RJF and other side fuels.

DFJ fermented sugars to a C15 alkene – farnesene [23,58], in a biphasic reactor (aqueous and organic phase). To achieve a 50% blend with fossil jet, farnesene must be hydrocracked [59,60] and then distilled [7].

Table 2
Summary of process conditions of fermentation and their energy products (EP) upgrade to renewable jet fuel.

Process variable	ETJ[h,i,m]		DFJ[j,n,o]	
T (°C)/P (atm)/time (h)/pH	33/1/8/5 [61]		30/1/not considered	
Operation mode of fermentation	Fed-batch anaerobic [62–64]		Continuous aerobic [19,23]	
EP final concentration (wt%)[a]	10 [22]		12.4 [23]	
Yields of fermentation (kg product kg^{-1} sugar inlet)	Glucose	Xylose	Glucose[k]	Xylose[l]
Ethanol[b]	0.460 [65]	0.435 [41]	–	–
Biomass[c]	0.031	0.023	0.060	0.060
Glycerol[d]	0.016 [66]	0.012 [66]	–	–
Xylitol[e]	–	0.047 [41]	–	–
Succinic acid[f]	0.008 [41]	0.012 [41]	–	–
Lactic acid[g]	0.030 [41]	0.030 [41]	–	–
Farnesene	–	–	0.236	0.236
Downstream EP recovery efficiency (%) and purity (wt%)	99.2%, 93.0 wt%		93.1%, 95 wt%	
EP upgrade to biojet	ETJ[p]		DFJ[q]	
H_2 input (kg H_2 kg^{-1} EP) & fraction reacted (%)	0.1 & 50% [67]		0.069 & 50% [19]	
Yields (wet kg dry kg^{-1} of EP)[r]				
LPG	0.033		0.480	
Naphtha	0.018		0.058	
Jet	0.523		0.434	
Diesel	0.064		0.070	
Water	0.155		0.259	

[a] Scenarios with WO and LHW designed in detail had final ethanol concentration, respectively, at 6.51 wt% and 7.64 wt% to guarantee lignin below inhibitory concentration. In scenarios with SS bagasse, these concentration are 1 wt% lower. For the same reason scenarios with alkaline, WO and LHW pretreatments had final farnesene concentration at ≈ 9.5% or 7.8% for LHW-A.
[b] $C_6H_{12}O_6 \rightarrow 2C_2H_6O + 2CO_2$ – 90% of glucose, $C_5H_{10}O_5 \rightarrow 1.67C_2H_6O + 1.67CO_2$ – 85% of xylose.
[c] $C_6H_{12}O_6 + 1.14NH_4^+ \rightarrow 5.71CH_{1.8}O_{0.5}N_{0.2} + 0.29CO_2 + 2.57H_2O + 1.14H^+$ – 4% of glucose, $C_5H_{10}O_5 + 0.95NH_4^+ \rightarrow 4.76CH_{1.8}O_{0.5}N_{0.2} + 0.24CO_2 + 2.14H_2O + 0.95H^+$ – 3% of xylose.
[d] H_2O extra reactant and O_2 side product [66] – 1.57% glucose and 1.18% xylose consumed.
[e] H_2O extra reactant and O_2 side product – 4.6% of xylose consumed [41].
[f] CO_2 extra reactant and O_2 side product - 0.6% of glucose and 0.9% xylose consumed.
[g] No extra reagent or side product – 3% of glucose and xylose consumed.
[h] Enthalpy of overall reactions (ΔHr) - 677.8 KJ kg^{-1}sugars [61].
[i] Biomass inoculum was at 10 wt% broth, NH_4OH was nitrogen source [63], and dispersant and antifoam were also considered, respectively, at 0.2 and 0.78 g L^{-1} [61].
[j] Mevalonate pathway has lower y_{sp} than MEP/DOXP one, respectively, 0.25–0.38 g g^{-1}, but was the one considered, as Amyris uses it [58].
[k] $C_6H_{12}O_6 + 0.09NH_4^+ + 0.91O_2 \rightarrow 0.22C_{15}H_{24} + 0.44CH_{1.8}O_{0.5}N_{0.2} + 2.27CO_2 + 3.06H_2O + 0.09H^+$ and $\Delta Hr = -2971.8$ kJ/kg glucose. 5% of $C_{15}H_{24}$ was considered a side-product.
[l] $C_5H_{10}O_5 + 0.07NH_4^+ + 0.76O_2 \rightarrow 0.18C_{15}H_{24} + 0.37CH_{1.8}O_{0.5}N_{0.2} + 1.89CO_2 + 2.55H_2O + 0.07H^+$ and $\Delta Hr = -2942.9$ kJ/kg xylose. 5% of $C_{15}H_{24}$ was considered a side-product.
[m] ETJ downstream included water scrubber [32] to recover EtOH from fermenters vent [41], biomass centrifugation, sterilization with 0.0126 kg H_2SO_4. kg^{-1} biomass and recycling [61] and distillation [32].
[n] DFJ downstream included three sequential centrifugations, a de-emulsification step with Triton X - 0.00282 kg kg^{-1} farnesene + side-product, a stabilization step with 1.17×10^{-4} kg *tert*-butyl catechol. kg^{-1} of farnesene + side-product [23].
[o] O_2 was input via an air stream, in excess - 1.88 mol O_2 inlet mol^{-1} O_2 reacted [23].
[p] EtOH dehydration and ethylene condensation to butylene followed stoichiometry, conversion and selectivity described in *Crawford* [57]. Each biofuel is a range of compounds but for simulation a single compound was chosen to represent LPG, naphtha, jet and diesel, respectively, pentene (C_5H_{10}), toluene (C_7H_8), *n*-dodecene ($C_{12}H_{24}$) and 1,14 – pentadecadiene ($C_{15}H_{28}$). Then, butylene oligomerization follows: $C_4H_8 \rightarrow 3.35 \times 10^{-3}C_5H_{10} + 0.0268C_7H_8 + 0.255C_{12}H_{24} + 0.0503C_{15}H_{28}$
[q] Farnesene hydrocracking: $C_{15}H_{24} + 0.35H_2 \rightarrow 1.15C_4H_{10} + 0.387C_5H_{12} + 0.16C_7H_8 + 0.58C_{12}H_{26} + 0.0153C_{15}H_{28}$ [19].
[r] Biofuels fractionation occurred through distillation with live steam input of 0.258 kg kg^{-1} of paraffin inlet and cuts following *Mayer* [19].

2.3.4. *Thermochemical upgrade of lignin and bagasse to biojet*

The main thermochemical processes for lignin and bagasse conversion and upgrading into biojet fuel are fast pyrolysis (FPJ), gasification Fischer-Tropsch (GFT), and Hydrothermal liquefaction (HTL). The most relevant advantages/disadvantages, process conditions and relative CAPEX are summarized in Section D.2 of SI [68–70]. FPJ and GFT are selected as the technologies for further analysis, where three types of lignin and two sources of bagasse are considered (see Table 3 and Table 4).

FPJ includes biomass conditioning and fast pyrolysis with gaseous phase recycling, from where bio-oil is recovered after quenching [71]. Bio-oil is then hydrotreated and deoxygenated, and the different biofuels are then recovered through distillation [70,71]. The heavy oil fraction is hydrocracked and again distilled to increase the biojet fuel yield (see Section E.2 of SI) [7,59].

GFT includes biomass conditioning, gasification (syngas with H_2/CO ratio above 2.1), syngas cleaning, H_2 SMR to reduce CH_4 in the outlet to 1.5%, and water gas shift (WGS) to adjust the H_2/CO ratio to > 2.2 [76], which favours waxes production in the Fischer-Tropsch reactor. Here, 70% of syngas is considered to be converted to a range of waxes which are then sent to hydroprocessing [76,77].

2.3.5. *Auxiliary sections*

The wastewater treatment section includes anaerobic treatment, where biogas is produced and then sent to H_2 SMR and aerobic treatment [41] (see Table 5). The sludge of both treatments is used for co-generation, after a concentration step. The supernatant undergoes reverse osmosis, which allows water recycling. H_2 SMR inlets included all the off-gas streams of biorefinery that contain CH_4 and/or H_2, and biogas from WWT and; if necessary due to unfulfilled energy requirements, natural gas is purchased. The H_2 SMR section includes desulfurization, SMR, pre-reforming, reforming and WGS [59]. Lower heating value (LHV) of each inlet stream, utilities properties and energy balance calculations of co-gen are summarized in Section E.3 of SI. The co-gen section includes conditioning of inlet streams and boiler, from where the high pressure (HP) steam produced is directly sent to the main processes or entered into the condensing extraction steam turbine (CEST) for medium pressure (MP), low pressure (LP) and electricity production. Flue gas leaving the boiler is used to pre-heat the inlet,

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Table 3
Summary of process conditions of lignin and bagasse upgrade to biojet fuel via fast pyrolysis.

Biomass type[a]	Lignin enzymatic hydrolysis [72,73]	Alkaline lignin [72,73]	High grade lignin [72,73]	SC bagasse [74]	SS bagasse [75]
Feedstock source	DA, SE, LHW	A	O, WO	Mills	Mills
Fast pyrolysis conditions [71]	T = 500 °C; T of sand = 605 °C; P = 1.5 bar; RT = 2 s; inlet moist. = 9%; sand/biomass = 14.5 kg kg^{-1}; fluidization gas/biomass = 3 kg kg^{-1}; fast pyrolysis quenching = 1.445 kg chilled water.kg^{-1} gaseous stream; flue gas recycled after quenching = 95%				
Bio-oil composition (kg kg^{-1} biomass (9% moist.) %) adapted from Refs. [72,73]					
Bio-oil frac.	**53.0**	**46.8**	**52.0**	**64.0**	**69.4**
phenolic	28.2	28.7	27.7	22.0	26.8
light ends	0.9	1.4	1.7	30.0	32.0
water	23.9	16.8	22.6	12.0	10.6
Non-condensable gas frac.	**13.0**	**14.9**	**14.3**	**19.0**	**17.2**
H_2	0.1	0.1	0.1	2.9	0.0
CO	6.4	7.3	7.0	9.0	5.1
CO_2	5.9	6.7	6.4	4.2	11.5
CH_4	0.7	0.7	0.7	2.9	0.6
Char frac.	**34.0**	**38.3**	**33.7**	**17.0**	**13.4**
H_2 input (kg H_2 kg^{-1} bio-oil) & fraction reacted (%) [59]	0.107 & 32% hydrotreating and 0.098 & 18% hydrocracking				
Hydrotreating & hydrocracking yields (wet kg. dry kg^{-1} biomass)[b]					
LPG	0.015	0.014	0.015	0.022	0.026
Naphtha	0.046	0.043	0.046	0.069	0.079
Jet	0.103	0.097	0.105	0.156	0.180
Diesel	0.083	0.078	0.084	0.124	0.144
Water	0.265	0.171	0.252	0.132	0.123

Bold numbers represent the total mass yield (in %) to the different fractions.
[a] Enzymatic hydrolysis lignin is attached to cellulose and hemicellulose which leads to higher bio-oil yield, but with higher water content; alkaline lignin is more recalcitrant, thus char yield is higher, however, phenolic content in bio-oil is higher [73].
[b] Yields presented for O and WO group correspond to lignin from WO. O results are ≈7% smaller. WO scenario includes the high grade lignin recovered with lignoboost but also the enzymatic hydrolysis slurry.

then it follows to the cleaning section [41].

2.4. Techno-economic assessment

Total purchase equipment cost (TPEC) of each process was based on estimations from previous publications (see Table 7). Furthermore, TPEC of liquid hot water and wet oxidation pretreatment technologies were based on the detailed designs and simulations. Adjustments of the equipment costs by capacity was based on the scaling up/down factors, while maximum allowed capacities and installation factors were retrieved from literature (see Table 7). Capital expenditure (CAPEX) of each scenario was

Table 4
Summary of process conditions of lignin upgrade to biojet fuel via gasification Fischer-Tropsch.

Biomass type	Lignin enzymatic hydrolysis	Alkaline lignin	High grade lignin
Source	DA, SE, LHW	A	O, WO[b]
Lignin elemental composition	[72]	Adapted from Ref. [72]	[78]
Gasification conditions [76]	T = 870 °C; P = 25 bar; inlet moist. = 9%; HP (high pressure) steam/biomass = 0.17 kg kg^{-1}; O_2/biomass = 0.26 kg kg^{-1}		
Syngas yields (kg kg^{-1} biomass (9% moist.) %)[a]	[79]	[80]	[46]
Syngas	58.6	52.8	47.4
H_2	39.2	33.0	41.0
CO	33.0	25.0	34.0
CO_2	12.1	36.0	10.0
CH_4	11.9	5.0	12.5
Other (C2-C4)	3.8	1.0	2.5
Solids [79]	29.6	29.6	29.6
Fischer Tropsch conditions[c] [76]	T = 200 °C; P = 25 bar;		
H_2 input (kg H_2 kg^{-1} hydrocarbons) & fraction reacted (%) [76]	0.06 & 100%		
Hydrotreating & hydrocracking yields (wet kg. dry kg^{-1} biomass)[d]			
Sulphur[e]	0.0004	0.018	0.0004
Naphtha	0.051	0.023	0.075
Jet	0.052	0.028	0.080
Diesel	0.047	0.038	0.086
Water	0.268	0.129	0.459

[a] Syngas and solids yields and composition were taken from literature, but liquid fraction was estimated: in all gasifications, moisture is 13.2% of outlet [76]; H_2S and NH_3 followed from the elemental composition of each lignin, respectively, S and N and tar was estimated to close mass balances.
[b] In WO and O there were two streams of lignin processed. The first is like enzymatic hydrolysis lignin (fraction not solubilized in pretreatment) and the second is the high end grade lignin, to which syngas yields are presented. Different proportion between the two explain biofuel yields for O ≈ 20% lower than for WO (the ones presented).
[c] Anderson-Schulz-Flory distribution of hydrocarbons considered for FT reactor: $(2n+1)H2 + nCO -> CnH(2n+2) + nH2O$, where $C_n = \alpha^{n-1}(1-\alpha)$ is the molar yield of a given carbon number n, α is the probability of chain growth and followed from *Martin* et al., [81]. α should be > 0.87 to maximize kerosene fraction.
[d] Fraction of hydrocarbons from FT reactor to each biofuel after hydroprocessing: naphtha – 100% of C5 to C8; jet –75% of C9, 100% C10 and C11, 50% of C12 to C16; diesel - 50% of C12 to C16, 100% C > 17 [82]. There is no LPG, because more volatile hydrocarbon produced in FT reactor followed to unreacted syngas stream sent to H_2 SMR section.
[e] Sulphur was produced from H_2S of syngas chelation in a LO-CAT column [76].

Table 5
Summary of process conditions of auxiliary sections: wastewater treatment (WWT), H_2 steam methane reforming (SMR) and co-generation (co-gen).

WWT	**Anaerobic**[a,b,c] [40] $COD_{eq} \rightarrow 0.21CO_2 + 0.23CH_4 + 0.06biomass + 0.5H_2O$	**Aerobic**[a,d] [40] $COD_{eq} \rightarrow 0.48CO_2 + 0.3biomass + 0.22H_2O$	Sludge concentration [41] Decanter and belt filter. 100% of sludge recovered at 32 wt%	Reverse osmosis [83] 75% of water recovered with 5 wt% of salts
H2 SMR	**PSA units in main sections** Non-reacted H_2 streams are recycled with 85% efficiency and 100% purity [60]	**Desulfurization** LO-CAT unit that allows 100% removal of NH_3 and H_2S (assumed)	**Reforming** [59] Pre-reformer: 3.5 mol steam mol^{-1} CH_4 SMR: 88% conversion of CH4 to syngas	**Water Gas shift**[e] [59] H_2/CO correction to 101 mol mol^{-1}
Co-gen	**Inlet streams concentration** [22] Filtration and drying until water < 45 wt%	**Boiler** 0.691 kg air MJ^{-1} LHV of the inlet; 87% efficiency [32]; boiler feed water vaporized to high pressure (HP) steam	**Condensing extraction steam turbine (CEST)** [84] Electricity produced with 90% efficiency; vacuum steam (TVS) turbine used to maximize electricity production	**Flue gas cleaning**[f] 2.45 kg of lime and 9.81 kg of water are used per ton of flue gas [41]

[a] Mass coefficients (kg kg^{-1} of chemical oxygen demand (COD) [85]) with 90% conversion [40].
[b] Biogas stream contains 98%, 0.5% and 100%, respectively, of CO_2, water and CH_4 [86].
[c] Non-digested waste and 75% of biomass at 2 wt% followed to decanter.
[d] Off-gas contained 98% and 0.17% of CO_2 and H_2O formed.
[e] After WGS, 98.7% of the water was condensed in a flash drum and 90% of the H_2 is recovered in a PSA unit.
[f] Solid waste produced from flue gas cleaning is transported, with associated cost (see Table 5 of SI), to landfill.

Table 6
Factors used for the economic analysis.

	Value
Plant lifetime (years)	15
Depreciation period (years)	10 [19,88,89]
Cost of capital (%)	12 [87]
Taxes in Brazil (%)	35 [19,88,89]
Equity (%)	100
Plant type	Greenfield, nth plant [6]
Plant capacity	100%

estimated using Guthrie's method [87].

Variable costs included raw materials and utilities (cooling water, chilled water, natural gas, sugarcane trash, and steam/electricity). Other operational costs, including fixed ones, were considered to estimate the operational expenditure of each scenario, following methodology of *Asselbergs* [87]. The Minimum jet fuel selling price (MJSP), which is the price at which biojet fuel must be produced to cover operational and capital expenses, was chosen for scenarios comparison since it allowed a direct comparison among scenarios and also to the fossil jet fuel prices.

Engineering Plant Cost Index (CEPCI) [90]. Adjustments on capacity were done considering the six-tenth rule when specific scale factors were not available for a particular equipment (see Table 21 (in Section E.4.) of SI). However, capacity limits were considered for most of the processes (see Table 7), meaning that a certain process might require multiple plants (rationale to determine number of plants is in section E.4.1 of SI).

Installation costs were also dependent on the technology considered (Table 7). CAPEX calculations were based on Guthrie's method which considers a Lang factor of 3.5 (advisable for mixed fluids and solids plants). Direct costs, which are 63% of the fixed capital investment (FCI), included TPEC, installation and other costs (*e.g.* land, buildings and structural buildings). Indirect costs, 37% of the FCI, included engineering, contractors fee and contingency. FCI was then corrected for location (a 10% factor) since most of the equipment indicators were from U.S. CAPEX included then FCI, working capital, which was 20% of sales revenue and start-up costs, which were 3% of the FCI.

Capital charge was the faction of CAPEX considered for minimum jet fuel selling price estimation. It was calculated as follows:

$$Capital\,Charge = \beta \cdot TCI \text{ where } \beta = \frac{i}{1-(1+i)^{-n}} \text{ is the capital charge factor}, i \text{ is interest rate} - 12\% - \text{and } n \text{ is project life} - \text{time}. \quad (1)$$

2.4.1. Economic factors

Factors used for the economic analysis were kept equal for all scenarios, as shown in Table 6. Greenfield integration level was considered, thus all scenarios consider stand-alone facilities, including auxiliary sections. An Nth plant system was considered, even though technologies included had different levels of maturity, and no additional development cost factors were considered [6]. On the other hand, a contingency factor, *i.e.* 13% of fixed capital investment, contemplated part of the risk from such innovative processes.

2.4.2. Total purchase equipment cost and capital expenditure

To estimate the TPEC of each scenario, reference data was taken from literature, adjusted to the year 2015 based on the Chemical

2.4.3. Variable costs and operational expenditure

Variable costs were estimated from the mass and energy balances. The former was used to determine the material inputs and their prices (see Table 5 in SI) while the latter was used as input to determine all the utilities requirements. Utilities requirements (*i.e.* steam, electricity, natural gas, cooling water, and chilled water) were calculated in detail (for WO and LHW pretreatments) from the energy balances -after applying heat integration- and also obtained from literature -under comparable conditions (see Table 8)-. In all cases steam and electricity are provided by the co-generation section. Furthermore, any sugarcane trash or natural gas required to guarantee enough energy input in the biorefinery were also included in the variable costs. OPEX was calculated based in *Asselbergs* method [87] (see Table 24 (Section E.4.2) of SI). Direct

Table 7
Limiting capacity, total purchased equipment cost (TPEC) and bare module installation costs (ISBL).

Section	Limiting capacity[c]	Units	TPEC (M $US\$_{2015}$)	ISBL (M $US\$_{2015}$)	Reference
Mills[a]	12,000	Wet SC ton day^{-1}	31.09	54.40	[20]
DA	3360	Wet bagasse ton day^{-1}	48.57	90.32	[22,40,41]
DA-A			71.96	135.85	[40,41]
SE			43.14	71.43	[22,41]
SE-A			67.74	119.38	[40,41]
ORG			83.87	166.09	[22,32,41]
WO[b]			54.05	99.06	[22,30,40,41,49,91]
WO detail			70.32	115.32	[32,41,92]
LHW			47.52	88.55	[22,40,41]
LHW-A			73.63	139.73	[40,41]
LHW detail			57.36	93.63	[41,92]
ETJ[d]	872	dry ton EtOH day^{-1}	32.73	57.16	[32]
ETJ-U[e]	2410		73.26	180.95	[93]
DFJ[f]	368	dry ton farnesene day^{-1}	31.18	39.37	[23]
DFJ-U[g]	3790		114.68	189.23	[7]
FPJ	2000	dry ton lignin or bagasse day^{-1}	79.27	212.73	[71]
GFT	2000	dry ton lignin day^{-1}	129.95	320.35	[91]
WWT[h]	41,233.1	ton wastewater day^{-1}	38.35	42.53	[40]
H_2 SMR	100	ton H_2 day^{-1}	26.75	51.35	[59]
Co-generation[i]	687.67	MW energy inlet of boiler	94.63	132.49	[22]
	125	MW electricity generated	43.71	73.87	[22]

[a] It was assumed that 25% of TPEC in *Dias* et al. ethanol biorefinery corresponded to milling [20].
[b] TPEC information for wet oxidation in literature only includes reactor pretreatment [49]. Therefore, combination of TPEC from other pretreatments was considered, including an ASU [91].
[c] Pretreatment limiting capacity is 2000 dry ton day^{-1} [22,41], but limitation used was assumed considering the bagasse yield obtained per each sugarcane mill.
[d] Ethanol fermentation capacity limitation - 174.4 kton dry EtOH yr^{-1} - was taken from *Humbird* et al., [41]. The maximum fermenter volume is 3900 m^3 [40].
[e] Ethanol upgrade capacity limitation – 482 kton yr^{-1}- was taken from *Atsonios* [5].
[f] Farnesene fermentation capacity limitation - 73.51 dry kton yr^{-1} – was taken from *Basto* [23] which corresponds to fermenter volume of 600 m^3.
[g] Limitation for farnesene upgrade was assumed similar to bio-oil hydroprocessing described in *Jones* et al. [59].
[h] No capacity limitation was considered for WWT. Capacity presented is the highest one obtained in one of the individual biorefinery scenarios.
[i] The heat/power ratio changes with each scenario, so TPEC of boiler and of extractive turbines have different reference capacities.

Table 8
Utilities requirements of each process section.

Section[a,b,c]	Electricity (kWh kg^{-1}x)	Steam (kg kg^{-1})			Cooling water (kg kg^{-1} x)	Chilled water (kg kg^{-1} x)	Natural gas (kg kg^{-1} x)
		LP	MP	HP			
Mills[d] [61]	0.012	0.181 ± 0.056	–	–	1.98	–	–
DA [40]	0.038 [41]	0.677	–	0.039	23.5	–	–
SE [40]	0.038 [41]	0.516	–	0.053	17.2	–	–
O [32]	0.069	0.376	0.350	0.552	33.4	–	–
WO [32]	0.077 [49]	0.376	0.026	0.552	18.6		–
WO detail[e]	0.006	–	0.055	0.159	59.9	1.46	–
LHW [40]	0.028 [41]	0.540	–	0.040	27.1	–	–
LHW detail[f]	0.003	0.051	0.359	0.189	125.1	2.67	–
ETJ [61]	0.113 [41]	2.470	–	–	80.3	1.82	–
ETJ-U [59]	0.143	–	0.154	–	5.30	0.921	0.016
DFJ	0.459	–	–	0.100	197.5[g]	–	–
DFJ-U	0.046	–	0.254	–	5.51	0.782	0.015
FPJ [59]	0.158 [95]	–	0.011	–	6.61	–	0.001
GFT [76]	0.265	–	0.007	0.177	18.2	–	0.003
WWT	0.5	–	–	–	–	–	–
H_2 SMR [59]	0.047	–	–	–	–	–	0.043

[a] x is kg wet feedstock for milling, kg wet bagasse for pretreatments, dry ethanol or farnesene for fermentation and upgrade sections, kg of dry lignin or bagasse for direct upgrade to jet, kg of COD inlet for WWT, kg of H_2 in the outlet of H_2 SMR.
[b] Pretreatments: 14% of the electricity in a bioethanol plant is consumed in pretreatment [41]; 20% of LP steam, 40% of HP steam and 20% of cooling water used in bioethanol production are consumed in pretreatment [40]. It was also included 10% of the total steam required in multi-effect evaporator, after heat integration assumed.
[c] It was assumed that alkaline treatment of bagasse does not increase utilities.
[d] LP steam spent in mills depended on the final concentration of the juice stream, which varies with each scenario. Result presented is an average with standard deviation and assuming that due to heat integration only 17% of the steam necessary was consumed.
[e] Results presented are after heat integration, which caused the following energetic saving: LP – 100%; MP – 89%; HP – 71%; CW – 33%; ChW – 77%.
[f] Results presented are after heat integration which caused the following energetic saving: LP – 82%; MP – 0.8%; HP – 80.5%; CW – 18%; ChW – 46%.
[g] Estimation based on the enthalpy of reaction and assuming that 50% reduction was possible.

production costs were about 50% of OPEX and included variable costs, labour costs (which change with type of process [94]), maintenance (equivalent to 5% of TPEC) and installation costs. Fixed costs, which are about 48% of OPEX, included local taxes, insurance and depreciation costs. About 2% of OPEX corresponded to general expenses (*i.e.* R&D and administration).

2.4.4. Minimum jet fuel selling price

To determine MJSP, it was necessary to calculate the OPEX (including the capital charge) and the sales revenue (including

Table 9
Overall jet fuel yield (kg jet/kg feedstock - %) for reference scenarios.

Overall jet fuel yield (kg jet kg^{-1} feedstock - %)										
Fermentation	Lignin dest.	Bagasse dest.								
		DA	DA-A	SE	SE-A	O	WO	LHW	LHW-A	FPJ
ETJ	FPJ	5.46	5.50	5.47	5.48	5.53	5.58	5.30	5.39	
	GFT	5.25	5.35	5.26	5.34	5.44	5.48	5.09	5.24	
	Co-gen	5.03	5.29	5.07	5.28	5.22	5.17	4.87	5.18	5.48
DFJ	FPJ	2.46	2.34	2.44	2.32	2.41	2.49	2.39	2.29	
	GFT	2.24	2.19	2.23	2.18	2.32	2.39	2.18	2.14	
	Co-gen	2.02	2.13	2.04	2.13	2.10	2.08	1.96	2.08	

those from selling all side products, *i.e.* other fuels, juice, lignin, acetic acid and furfural).

2.4.5. Sensitivity analysis

MJSP results had an uncertainty which is a consequence of the wide combination of references and also of a few assumptions. A list of parameters with large influence on the economic performance is selected for all scenarios to analyse their effect on the MJSP, they are: feedstocks and SC trash price; TPEC of auxiliary sections (i.e. WWT and co-gen); TPEC of thermochemical technologies (*i.e.* ETJ-U and FPJ); jet fuel overall yield from both SS and SC, and crude oil price. In all cases, optimistic and pessimistic conditions are identified with respect to the reference values. For the case of crude oil price, pessimistic conditions refer to low selling prices for all side products (as defined by the crude oil price) while the optimistic conditions refer to higher selling prices for all side products (allowing a lower MJSP) at a level such that the selling price of all products (biojet fuel and side products) are just competitive with the crude based counterpart.

2.5. Environmental assessment

The environmental analysis includes calculations for greenhouse gas (GHG) emissions and for non-renewable energy use (NREU) in a cradle-to-gate + combustion system boundaries. However, emissions from valorisation processes of both juice (to succinic acid) and lignin (to polyurethane) were not included. Furthermore, the system expansion approach was considered for electricity production, with the Brazilian electricity mix used as reference. Since the SC RJF biorefinery is a multiproduct system, three allocation methodologies were compared: mass, energy and economy. The total GHG emissions and primary energy use impacts were then accordingly allocated to each product by their mass flowrate, lower heating value (LHV) or price [96]. Individual environmental impact factor per type of process input (*e.g.* raw materials, feedstocks, and utilities) are included in Table 25 (Section E.5) of SI.

3. Results and discussion

3.1. Process design and economic assessment of reference scenarios

In the mills, 280 kg of bagasse and 145 kg of juice were obtained per ton of SC. These results are in line those previously published by other authors [65]. The performance of different pretreatments, fermentation and lignin upgrade is compared in Table 27 (Section F.1) of SI. Fermentable sugars (glucose and xylose) yield obtained was higher for alkaline pretreatments, especially when lignin is used in co-generation (see Table 9). Non-hydrolysed biomass stream recovered after enzymatic hydrolysis was sent to lignin

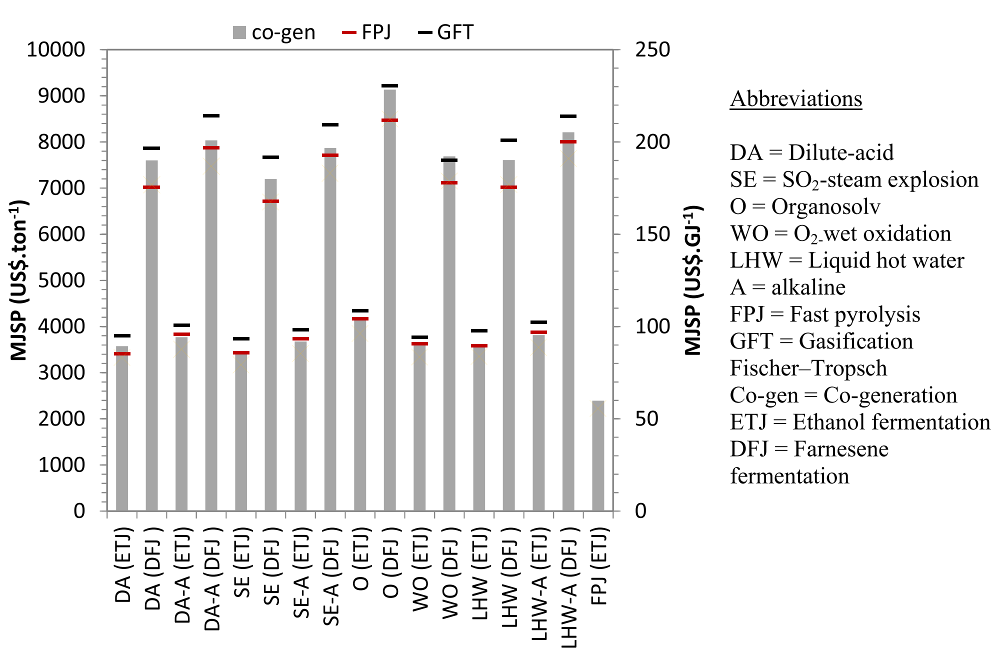


Fig. 2. Minimum jet fuel selling price (MJSP) of reference scenarios (all juice used for jet fuel production, all lignin is used for jet fuel production or co-generation and hemicellulose hydrolysate stream is detoxified).

Table 10
Specifications of new scenarios with process improvement options.

Group	Feedstock	Pretreatment	Fermentation	Lignin destination	Bagasse destination	Key improvements
A	SC	WO detailed	ETJ	Polyurethanes	Pretreatment	heat and water integration + acetic acid and furfural recovery based on Aspen Plus simulation
		LHW detailed		Co-gen		
B	SC	DA	ETJ	Co-gen	Pretreatment	30.2 kton juice yr^{-1} for succinic acid production
		SE				
		WO detailed		Polyurethanes		
		LHW detailed		Co-gen		
C	SC + SS	DA	ETJ	Co-gen	Pretreatment	Operation time increased to 320 days
		SE		Co-gen		
		WO detailed		Polyurethanes		
		LHW detailed		Co-gen		
		None		None	FPJ	

Table 11
Overall jet fuel yields for scenarios with improvement options.

Scenario group	A, B		C				
Feedstock	SC		SS				
Bagasse destination	WO detail	LHW detail	DA	SE	WO detail	LHW detail	FPJ
Jet fuel yield (kg jet kg^{-1} feedstock - %)	5.25	4.99	4.23	4.27	4.45	4.20	4.99

thermochemical upgrade only when its dry lignin content is above 50%, otherwise it followed to co-generation. Ethanol yield slightly differs with the pretreatment from which sugars 2G were obtained, as consequence of different proportion between C6 and C5 sugars and the fact that ethanol yield is lower for C5 [41]. Both farnesene fermentation and upgrade yields were significantly lower when compared to ETJ which causes an overall jet fuel yield half of the one obtained with ethanol. FPJ of bagasse led to a jet fuel yield ≈50% higher compared to the one obtained with lignin FPJ. Organosolv, wet oxidation and bagasse FPJ led to the highest overall jet fuel yields (see Table 9).

Fig. 2 shows the MJSP of all reference scenarios. The ones with farnesene fermentation had an MJSP almost twice higher than those of ethanol fermentation as consequence of the lower overall jet fuel yield of DFJ compared to ETJ (*i.e.* 24 and 54 kg jet ton^{-1} SC, respectively). The lower RJF yield led to higher feedstock and raw materials expenses and consequently higher capital investment (see Table 28 (Section F.1) of SI for MJSP contributions). This relation of MJSP with the fermentation pathways has been previously reported [6,8,97].

Bagasse FPJ led to the lowest MJSP among all studied scenarios as consequence of: *i*) reduction of raw materials expenses and capital investment costs (*i.e.* 75% and 15% respectively); and *ii)* an increase of 50% in revenues from side fuels sales -compared to ETJ scenarios with pretreatment-. Thermochemical conversion of lignin to jet via FPJ reduced the MJSP by 2% for alkaline lignin, and by 7% for lignin from other pretreatments due to: increased overall jet fuel yield, increased sales revenues and lower external demand of utilities. In contrast, GFT upgrade of lignin caused an increase in the MJSP due to its extra capital investment. Dependency of MJSP for different pretreatments is maintained in either DFJ or ETJ scenarios. In both fermentation scenarios, lower MJSP was achieved for DA and SE followed by WO and LHW. Alkaline pretreatment caused an increase in capital investment of pretreatment and a dilution of waste streams which resulted in higher WWT capital investments. As consequence, such scenarios had higher MJSP even though they also had higher overall jet fuel yield. In the case of organosolv, the higher operational costs (*i.e.* solvent purchase) and capital investment explain the increased in the MJSP.

Since none of the scenarios reported a MJSP close to the price of fossil jet fuel, three process improvements are considered to enhance the economic performance of the scenarios. A list of the new scenarios is shown in Table 10 (and Figure 5 (Section F.2.) of SI). In this new list of scenarios, the non-hydrolysed biomass was used only in the co-generation system since its upgrade to jet via FPJ added complexity to the biorefinery without much benefits for the MJSP. In the WO scenario, lignin was considered to be sold to polyurethane manufacturing. The juice sold in group B (see Table 10) was such that it covers 5% of the global biosuccinic acid (bSA) demand in 2020, *i.e.* 42.3 bSA kton yr^{-1} [98–100]. During the SS use period, group C, no SC trash is available, thus, energy from provided by the co-generation system was covered by natural gas.

3.2. Process design and economic assessment of groups A, B and C

Overall, jet fuel yield in group A was about 2% higher than the corresponding reference scenarios as consequence of the increased sugars 2G yield (see Table 30 (Section F.2) of SI). SS bagasse pretreatments and FPJ yields were higher than the corresponding ones for SC. Nevertheless, the overall jet fuel yield when SS is used was 15% lower than that for SC since juice extracted in SS milling was lower by 23% (see Table 11). Overall, jet fuel yield of group B scenarios was the same as the reference scenarios or as those from group A; however, there is extra feedstock requirements (≈3.5%) to cover the same jet fuel demand (see Table 31 (Section F.2) in SI). Scenarios with pretreatment had the highest feedstock requirements, approximately 4400 kton yr^{-1} of SC or 1680 kton yr^{-1} of SS meaning that 1.3% of total SC produced in São Paulo state or 22.4% of current SS produced in Brazil would be necessary (see Table 1 of SI).

Fig. 3 shows the different contributions to MJSP for the reference scenarios with the best economic performance, and also includes the MJSP contributions for scenarios of groups A, B and C. All improvement options led to reduced MJSP, however none of the

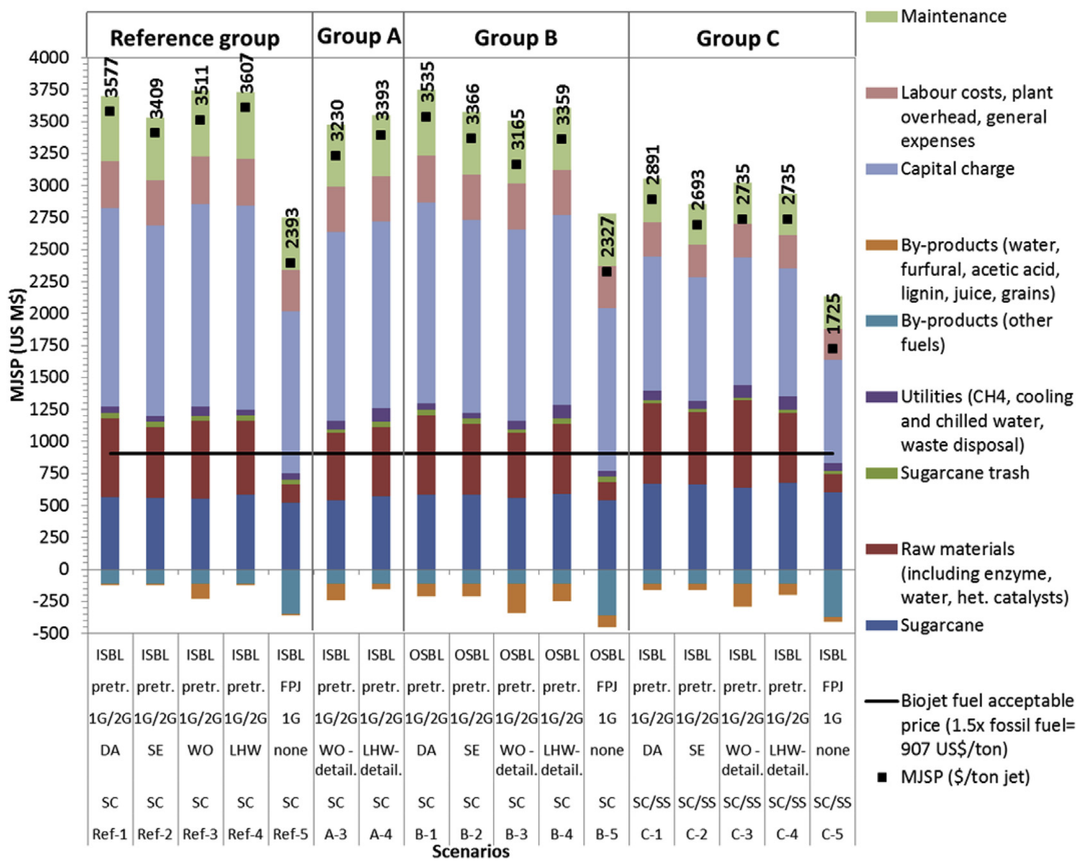


Fig. 3. Costs contribution to the minimum selling price of biojet fuel for main cases of reference scenarios and for groups A, B and C (at: crude oil price of 64.56 US\$.barrel^{-1}; sugarcane juice price of 632 US\$.dry ton^{-1}; and lignin price of 400 US\$.dry ton^{-1}).

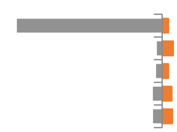
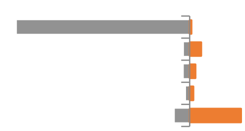
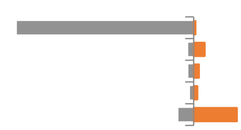
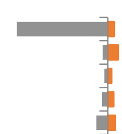
scenarios reached biojet fuel prices that are comparable to those of the fossil jet fuel or acceptable for a biobased fuel [101]. In most cases, capital charge was responsible for approximately 50% of biojet fuel selling price, which is the reason why the best scenarios in terms of CAPEX (see Table 32 (Section F.2) of SI) were also the best in terms of MJSP. Increasing the operation time to 320 days per year reduced the daily capacity, and in consequence the CAPEX, leading to the scenarios of group C to have the lowest MJSP. In this group C, the MSJP was reduced by ≈ 15% and ≈30% for scenarios with bagasse pretreatment or direct upgrade to jet, respectively. The larger reduction of MJSP for scenarios with bagasse FPJ was due to a combination of smaller daily capacity with higher overall jet fuel yield that reduced number of plants required. Such plants operate at capacities closer to their maximum, and therefore, they benefit from the economy of scale effect. Moreover, the yield of the other biofuels co-produced was higher in scenarios with bagasse FPJ. In group A, TPEC of pretreatments designed in detail was higher than corresponding ones in the reference scenarios per unit of bagasse used; however the MJSP was around 8% lower. This reduction in the MJSP was a consequence of: *i)* a slightly higher overall biojet fuel yield (reducing the mills and pretreatment required processing capacities); *ii)* the extra revenues from selling acetic acid and furfural; and *iii)* the improved integration of energy and water (reducing the CAPEX of the co-gen and WWT systems). In group B, selling sugars improved the gross profit by 16%, but the MJSP was only reduced by 2% when compared to the respective reference scenarios and to group A. This small reduction in the MJSP was a consequence of the increased sugarcane and capital requirements which is not sufficiently compensated by the extra sales revenues.

3.2.1. Sensitivity analysis

This section analyses the effects of the parameters with the largest contributions to MJSP on the economic performance of key scenarios. For example, CAPEX is responsible for around 50% of MJSP (see Fig. 3) where auxiliary sections (*i.e.* WWT and co-gen) are the major contributors followed by the thermochemical technologies (*i.e.* ETJ-U and FPJ). Feedstocks and SC trash prices are, on the other hand, the largest shares of OPEX. Two additional parameters with large influence on the MJSP and economic competitiveness of biojet fuel are the overall yield on feedstocks (*i.e.* SS and SC) and the reference price for crude oil. Table 12 shows the variability of the MJSP with respect to these parameters above mentioned.

Results show that the largest reductions to the MJSP are achieved when higher selling prices are possible for all side products. This situation may be possible under two different cases: *i*) high crude oil prices (resulting in competitive higher selling prices for the biobased side products); and *ii*) premium selling prices applicable to all side products from the biojet fuel production biorefinery system. In the latter case, the price gap (between the fossil based and the biobased products) could be reduced by different policies such as carbon fees, subsidies or tax exemption. All the other parameters, *i.e.* technological (overall biojet fuel yield from SS/SC) and economic ones (feedstocks and SC trash price, TPEC of auxiliary sections, and TPEC of thermochemical technologies), showed to have relatively minor effects on the potential reduction of the MJSP. It is worth to notice that the three alternatives options defined for the reference scenarios (*i.e.* recovery of by-products, valorisation of sugars and lignin streams, and increase of operation time by using a cumulative feedstock) have larger effects on the reduction of the MJSP (see Table 12). Thus, when all appropriate conditions are

Table 12
Sensitivity analysis of most promising cases to produce jet fuel.

Scenario	Parameter	Optimistic	Base	Pessimistic	MJSP variation
Ref1-SE-ETJ	Crude oil price (US$.bbl^{-1})[b]	151.61	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	79.81/112.2	+10	
	TPEC of ETJ-U/FPJ (US M$)	−10%	105.3/0	+10	
	Jet fuel yield (kg jet.ton-1 SC)[a]	54.0	50.7	47.4	
A3-WO detail.-ETJ	Crude oil price (US$.bbl^{-1})[b]	147.57	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	77.0/92.5	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	105.3/0	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	56.0	52.5	49.0	
Ref5-FPJ-ETJ	Crude oil price (US$.bbl^{-1})[b]	121.74	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	41.1/80.1	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	70.7/115.8	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	57.5	54.8	52.0	
B2-SE-ETJ-OSBL	Crude oil price (US$.bbl^{-1})[b]	150.65	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	80.4/113.9	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	105.3/0	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	54.0	50.7	47.4	
B3-WO detail.-ETJ-OSBL	Crude oil price (US$.bbl^{-1})[b]	146.08	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	79.0/94.0	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	105.3/0	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	56.0	52.5	49.0	
B5-FPJ-ETJ-OSBL	Crude oil price (US$.bbl^{-1})[b]	119.91	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	40.6/81.0	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	69.7/118.4	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	57.5	54.8	52.0	
C2-SE-ETJ-SC/SS	Crude oil price (US$.bbl^{-1})[b]	134.72	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	48.3/68.8	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	73.0/0	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	54.0/45.7	50.7/42.7	47.9/39.8	
C3-WO detail.-ETJ- SC/SS	Crude oil price (US$.bbl^{-1})[b]	135.79	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	46.5/57.8	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	73.0/0	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	56.0/47.7	52.5/44.5	49.0/41.4	
C5-FPJ-ETJ- SC/SS	Crude oil price (US$.bbl^{-1})[b]	103.29	64.5	52.39	
	Feedstock/trash price (US$.ton^{-1})	−10%	22.28/16.90	+20%	
	TPEC of WWT/co-gen (US M$)	−10%	24.5/48.2	+10%	
	TPEC of ETJ-U/FPJ (US M$)	−10%	46.2/68.7	+10%	
	Jet fuel yield (kg jet.ton-1 SC)[a]	55.8/52.3	54.8/49.9	52.0/47.4	

[a] Changes in biojet fuel yield are limited to increasing/decreasing in 5% sugar yield in pretreatments or jet fuel yield in ethanol or bagasse thermochemical upgrades.
[b] Optimistic scenario crude oil price was derived from selling all biofuels produced (LPG, naphtha, jet and diesel) with the same premium fee (as compared to fossil based prices).

combined (see bagasse FPJ in a SC/SS biorefinery scenario in Table 12), the resulting MJSP is only 1.6× above the current fuel price (605 US$.ton^{-1}).

3.3. Environmental assessment

Fig. 4 shows the GHG emissions and NREU considering the three allocation methods, *i.e.* mass, energy and economy, for the most relevant cases of the reference scenarios and of the improved scenarios (groups A, B and C). Different allocation methods led to, for each scenario and environmental impact category, comparable results. The main contributions to GHGs and NREU, for scenarios with pretreatment were from pretreatment (40 and 65%, respectively), co-generation (35 and 15%) and feedstock growth/harvesting/transportation (25 and 20%). Both GHGs and NREU should lead to, at least, 50% reduction of environmental impacts as compared to the fossil jet fuel emissions, which are 85 kg CO_2 GJ^{-1} [10] and 1200 MJ GJ^{-1} [102] respectively. Scenarios with thermochemical conversion of bagasse were steadily below the emission targets because of higher biojet fuel yield (resulting lower raw materials requirements), lower requirements of inorganic compounds (acids/bases used in pretreatment for pH correction) and lower energy consumption. On the other hand, ETJ pathways led to comparatively higher GHG emission than the thermochemical routes [10,102]. The fact that a large fraction of the GHG emissions are originated from the pretreatment step explains the higher emissions compared to 1G biojet fuel production via the ETJ process from sugarcane, 12.9 kg CO_2 GJ^{-1} [97]. Scenarios with sugars as co-

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Fig. 4. Greenhouse gas (GHG) emissions and Non-renewable energy use (NREU) of key cases for reference scenarios and for group A, B, and C.

products led to lower emissions due to the higher allocation factor on the sugars stream. Scenarios combining the two feedstocks (SC and SS) had higher emissions since *i)* the biojet fuel yield from SS is lower (indicating a higher feedstock and raw materials requirement) and *ii*) additional natural gas was used for heat generation. GHG emissions and NREU for the other biofuels co-produced were calculated to be in the same range as those range of the biojet fuel (see Tables 34 and 35 (Section F.2) of SI for results considering mass allocation).

4. Conclusions

Clear conclusions regarding preferred technologies for biojet fuel production were obtained in this project: *i*) ethanol fermentation is considerably more economic than the farnesene route; *ii)* upgrading lignin to biojet increases complexity without major reductions on the MJSP; and *iii*) bagasse should be upgraded to biojet via fast pyrolysis instead of undergoing the pretreatment pathway. The latter case, *i.e.* bagasse FPJ, led to the lowest MJSP among all considered scenarios due to a combination of higher overall biojet fuel yield and its related lower capital requirements. Furthermore, the MJSP of the bagasse FPJ and juice ETJ cases can be further reduced by using SS as cumulative feedstock which increases the active period of the facilities and also reduces the processing capacity for a given annual production. In the case of SC bagasse pretreatment routes, the WO and SE pretreatment options are preferred with acetic acid and furfural recovery.

Furthermore, even when premium fees were considered for all biofuels produced in the biorefinery, an integrated 1st and 2nd generation biojet fuel production from sugarcane did not reach a minimum selling price competitive with current fossil jet fuel price.

In terms of environmental impacts, most scenarios led to GHG emissions and NREU values that are around the expected 50% reduction as compared to those from fossil based jet fuel. Finally, the best economically performing scenario is SC juice ETJ and bagasse FPJ biorefinery, which also had the lowest environmental impacts.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.renene.2017.05.011.

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