Production of Sustainable Aviation Fuels from Lignocellulosic Residues in Brazil through Hydrothermal Liquefaction: Techno-Economic and Environmental Assessments

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Supplementary Material

1. Biomass Characterization

Table S1. Biomass characterization

Composition (weight %, dry basis)	Sugarcane Bagasse[a]	Sugarcane Straw[b]
Carbon	46[c]	45.6[c]
Oxygen	44.5[c]	43.9[c]
Hydrogen	5.8[c]	5.7[c]
Nitrogen[d]	0.6[d]	0.5[d]
Sulphur[d]	0.1[d]	0.1[d]
Chlorine	0.02[d]	0.1[d]
Ash	2.9[c]	4.1[c]
Moisture	50[c]	15[c]
HHV, MJ/kg, dry basis	18.3	18
LHV, MJ/kg, dry basis	16.8	16.7
LHV, MJ/kg, dry and ash free basis	17.4	17.3

a. Including mineral and vegetal impurities.

b. Composition for baled straw.

c. Carbon, oxygen, hydrogen, ash and moisture content of bagasse and straw and the were calculated from the Virtual Biorefinery database [1].

d. Data from [2].

2. Heat and power parameters for HTL plant

The heat and power data necessary for the HTL plant was obtained from a previous study issued by the laboratories of the Department of Energy of the United States. This data is showed in Table S2. Tews et al. has reported the techno-economic analysis of woody conversion into HTL biofuels, providing a complete data set on the mass and energy balances generated from Aspen simulation models. Thus, this available data was used for the calculation of sugarcane HTL, and small adjustments were made, when necessary, as detailed in the Table S2. The specific data concerning the yields obtained from sugarcane bagasse was retrieved from an experimental study which investigated the conversion of this biomass utilizing two different solvents: water and ethanol [3]. As sugarcane bagasse and straw have very similar composition, and there is no experimental study of HTL of sugarcane straw in the literature, the available date on HTL for sugarcane bagasse was used as a proxy for sugarcane straw. Similarly to [4], the present study has assumed that the off-gases (except CH_4) and bio-char produced as HTL by-products were burned to provide heat to the process. The methane in the off gases was employed as input for the hydrogen plant, but as it amounted to small volumes, additional natural gas was externally purchased. The mass and energy balances for a methane steam reforming hydrogen plant was retrieved from [5]. The hydrotreating of the HTL bio-crude was assumed to be comprised of two stages: the first stage had a mild severity targeting the stabilization of the bio-crude and the second with higher severity to promote mainly the deoxygenation of the bio-crude.

Table S2. Heat and power factors for the calculation of mass and energy balances of HTL

Section	Unit	EtOH Value	H2O Value	Reference
BIOMASS PREPROCESSING				
Grinding energy	kWh/kg dry B	0.0712	0.0712	[4]
Handling, dust collection	kWh/kg dry B	0.005	0.005	[4]
PUMPING				
Inlet pressure	bar	1	1	Assumed
Outlet pressure	bar	165	165	[6]
Solid/Solvent Ratio	wt.	0.2	0.2	Assumed
Electricity consumption	kWh/kg dry B	0.0462	0.0462	[4]
CONVERSION & HEAT RECOVERY				
Inlet temperature	°C	300	300	[3]
Electricity consumption	kWh/kg slurry	0.0089	0.0089	[4]
Yield (of dry biomass)				
Biocrude	wt.	0.483	0.409	[3]
Solids	wt.	0.258	0.292	[3]
Gas	wt.	0.193	0.040	[3]
Aqueous	wt.	0.067	0.259	[3]
Biocrude				
Moisture	wt.	0.05	0.05	[4]
Organics	wt.	0.95	0.95	[4]
Off-gases				
CO2	wt.	0.902	0.902	[4]
H2	wt.	0.009	0.009	[4]
C2H6	wt.	0.025	0.025	[4]
C3H8	wt.	0.019	0.019	[4]

C4H10	wt.	0.015	0.015	[4]
CH4	wt.	0.03	0.03	[4]
Heat exchange efficiency	%	80	80	Assumed
Heat consumption (to heat the inlet stream)	MJ/kg inlet	0.73	1.08	Calculated
Heat consumption (to keep reactor isothermal)	MJ/kg inlet	0.124	0.124	[7]
Water heat capacity	MJ/kg	-	0.00418	(NIST Webbook,2021)
Bagasse heat capacity	MJ/kg	0.00297	0.00297	[8]
Ethanol heat capacity	MJ/kg	0.00257	-	(NIST Webbook,2021)
SOLVENT RECOVERY				
Heat consumption (steam to evaporate solvent)	MJ/kg inlet	0.11	-	Calculated
Ethanol recovery efficiency	%	90	-	Assumed
HYDROTREATMENT AND DISTILLATION				
Hydrotreater				
Inlet temperature	°C	165	165	[4]
Inlet pressure	bar	136	136	[4]
Conversion temperature	°C	400	400	[4]
H2/biocrude ratio	kg H2/kg BCO	0.035	0.035	[4]
Number of stages	-	2	2	[9]
LHSV 1st stage fixed bed reactor	v/v/h	0.54	0.54	[9]
LHSV 2nd stage fixed bed reactor	v/v/h	0.18	0.18	[9]
Catalyst type	-	Co-Mo/Al2O3	Co-Mo/Al2O3	[10]
Catalyst density	kg/m3	1201	1201	[11]
Catalyst lifetime	y	1	1	[4]
Electricity consumption	kWh/kg BCO	0.069	0.069	[4]
Heat consumption (steam for the distillation columns)	MJ/kg	0.353	0.353	[4]
Yield (of bio-crude oil, in natura)				
Hydrotreated oil	wt.	0.75	0.66	[4]
Water	wt.	0.18	0.27	[4]
Off gas	wt.	0.07	0.07	[4]

Hydrotreated oil to final products				
Gasoline	wt.	0.3	0.3	[6]
Diesel	wt.	0.15	0.15	[6]
Jet fuel	wt.	0.5	0.5	[6]
Marine	wt.	0.05	0.05	[6]
Off gases				
H2	wt.	0.078	0.078	[4]
C2H6	wt.	0.151	0.151	[4]
C3H8	wt.	0.132	0.132	[4]
C4H10	wt.	0.049	0.049	[4]
C5H12	wt.	0.015	0.015	[4]
C6H14	wt.	0.393	0.393	[4]
CH4	wt.	0.182	0.182	[4]
HYDROGEN PRODUCTION				
Natural gas feedstock (@94.5% mol CH4)	kg NG/kg H2	3.12	3.12	[12]
Fuel (to fire the reformer, @94.5% mol CH4)	kgNG/kgH2	0.34	0.34	[12]
Steam requirement @2.6MPa/380 psi	kg steam/kg H2	10.29	10.29	[12]
Steam production (excess) @4.8MPa/700psi	kg steam/kg H2	14.78	14.78	[12]
Electricity consumption	kWh/ kgH2	0.42	0.42	[13]
GHSV	h-1	4000	4000	[4]
Catalyst type	-	NiMo	NiMo	[12]
Catalyst density	kg/m3	1201	1201	[11]
Catalyst lifetime	y	3	3	[4]
Hydrogen purity	mol% H2	>99.95	>99.95	[12]
UTILITIES				
Boiler efficiency (gas)	%	75	75	Industrial communication
Boiler efficiency (char)	%	50	50	Industrial communication
Fired Heater efficiency (gas, indirect heating)	%	75	75	Industrial communication
Fired Heater efficiency (char, indirect heating)	%	50	50	Industrial communication

Air excess (combustion)	%	20	20	[11]
Off-gases lower heating value	MJ/kg	41.1	41.3	[3]
Bio-char lower heating value	MJ/kg	15.4	16.7	[3]
Cooling water makeup	L/L product	9.44	9.44	[9]
Boiler feed water makeup	L/L product	0.96	0.96	[9]

Abbreviations: B= Biomass, BCO= biocrude oil

3. Mass fluxograms of the evaluated scenarios

The mass flows for each of the evaluated scenarios are showed in Figure S3-S7. The processes in the fluxogram with brow border are related to 2G (HTL) and the processes with green border are related to 1G (ethanol distillery). 1G process operates during sugarcane season (200 days), and the 2G operates for 330 days. Therefore, a storage of sugarcane bagasse was considered to allow the round year operation of HTL process. A storage of ethanol was also considered within the scenarios that utilize ethanol as solvent for liquefaction.

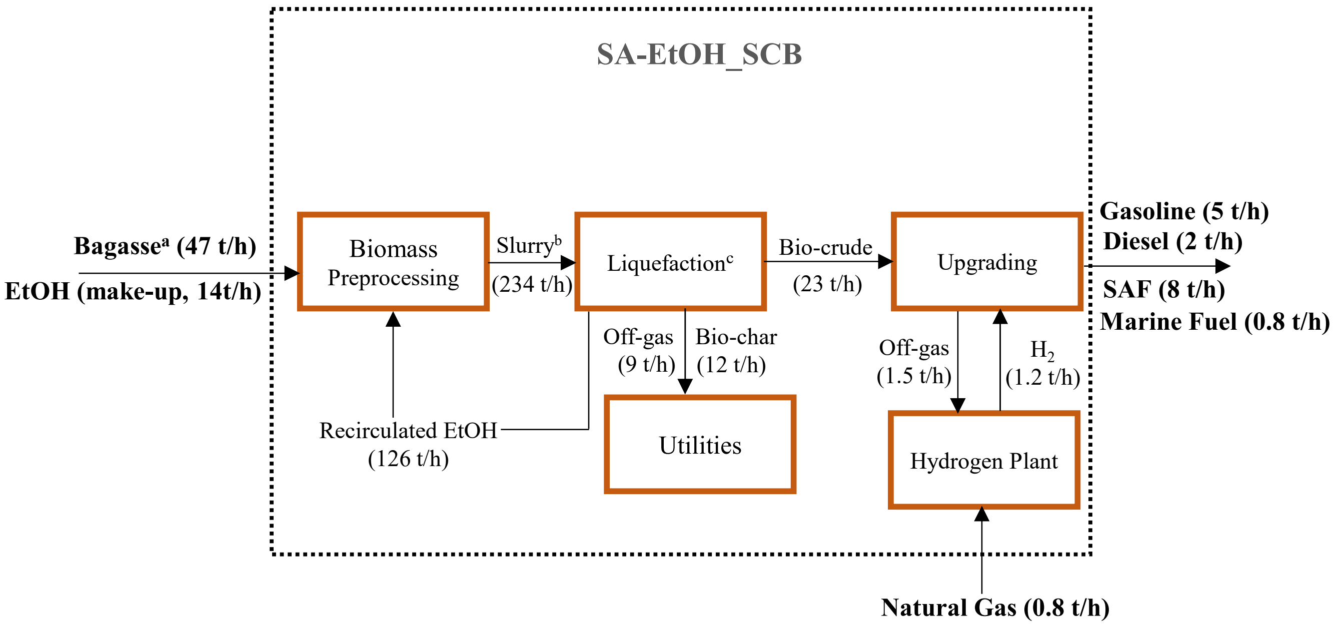

Figure S1. Mass fluxogram of SA-EtOH_SCB

a: Bagasse mass given in dry basis.

b: The bagasse moisture was accounted for in the slurry.

c: Liquefaction and Products Separation.

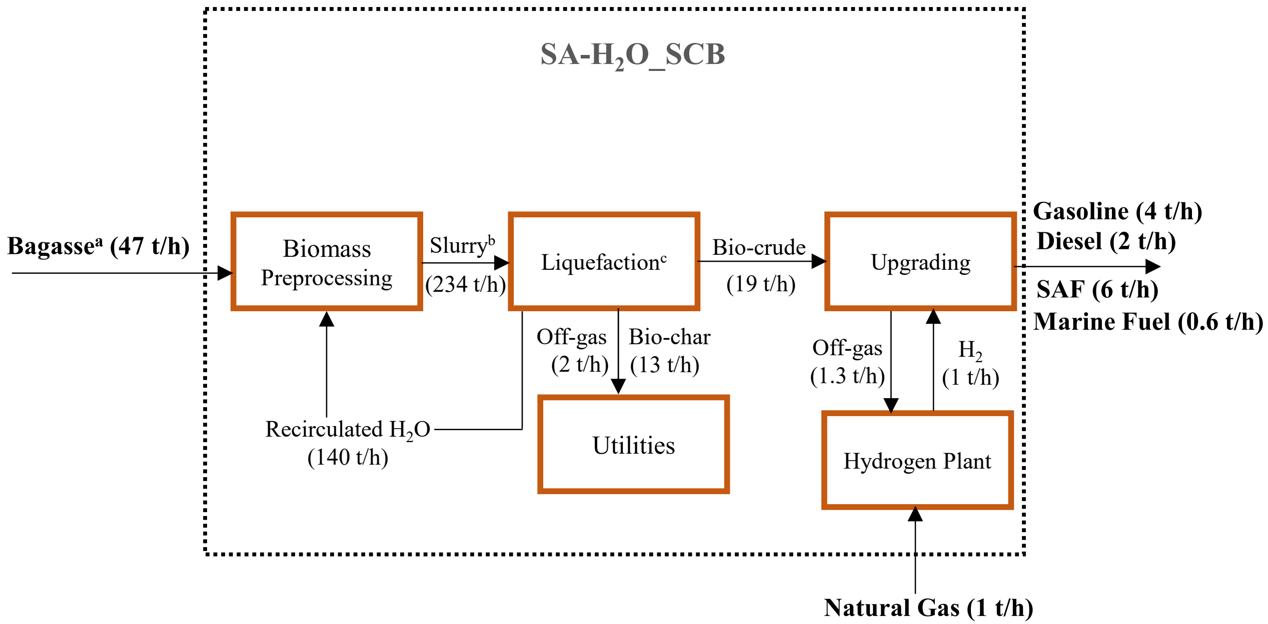

Figure S2. Mass fluxogram of SA-H_2O_SCB

a: Bagasse mass given in dry basis.

b: The bagasse moisture was accounted in the slurry.

c: Liquefaction and Products Separation.

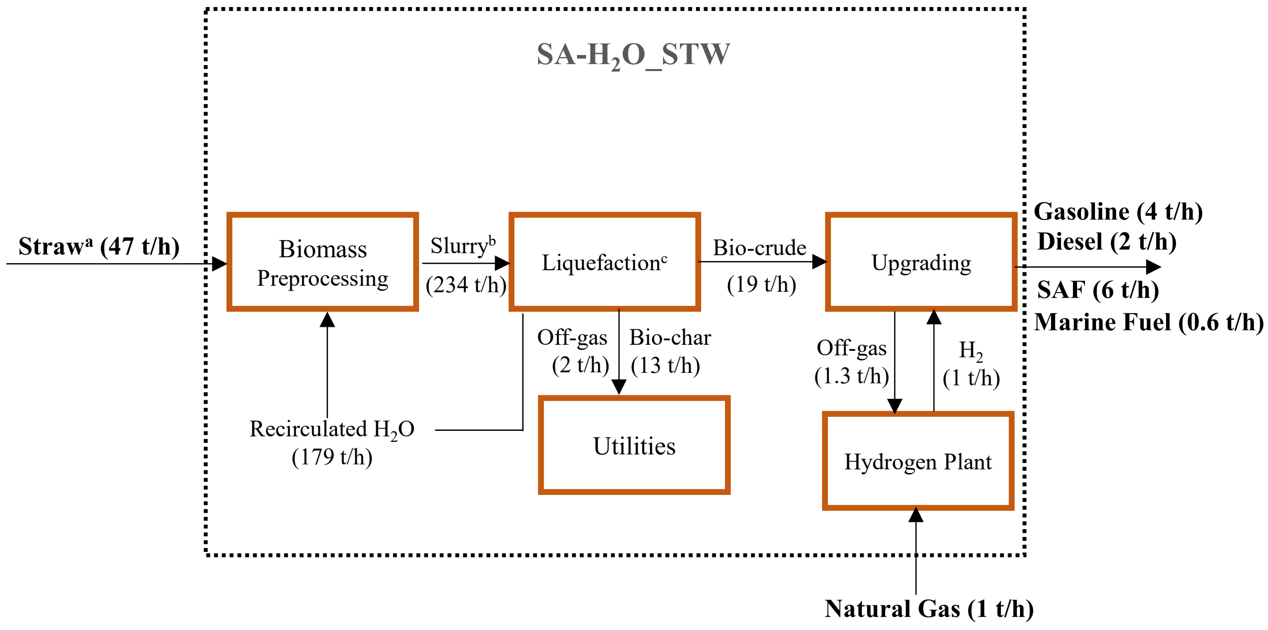

Figure S3. Mass fluxogram of SA-H_2O_STW

a: Straw mass given in dry basis.

b: The straw moisture was accounted for in the slurry.

c: Liquefaction and Products Separation.

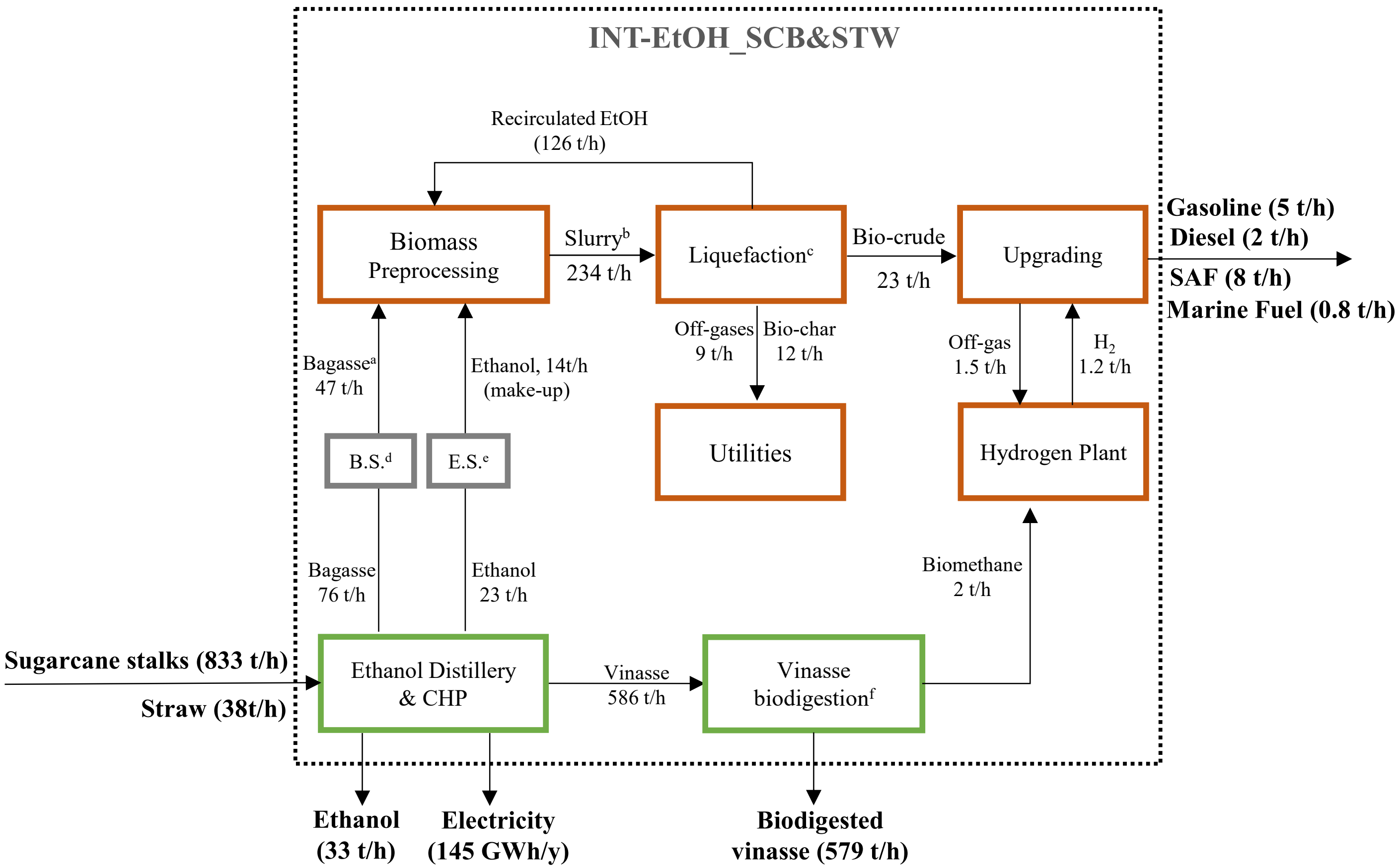

Figure S4. Mass fluxogram of INT-EtOH_SCB&STW

a: Bagasse mass given in dry basis.

b: The bagasse moisture was accounted for in the slurry.

c: Liquefaction and Products Separation.

d. Bagasse Storage.

e. Ethanol Storage.

f. Vinasse Biodigestion & Biomethane Upgrading

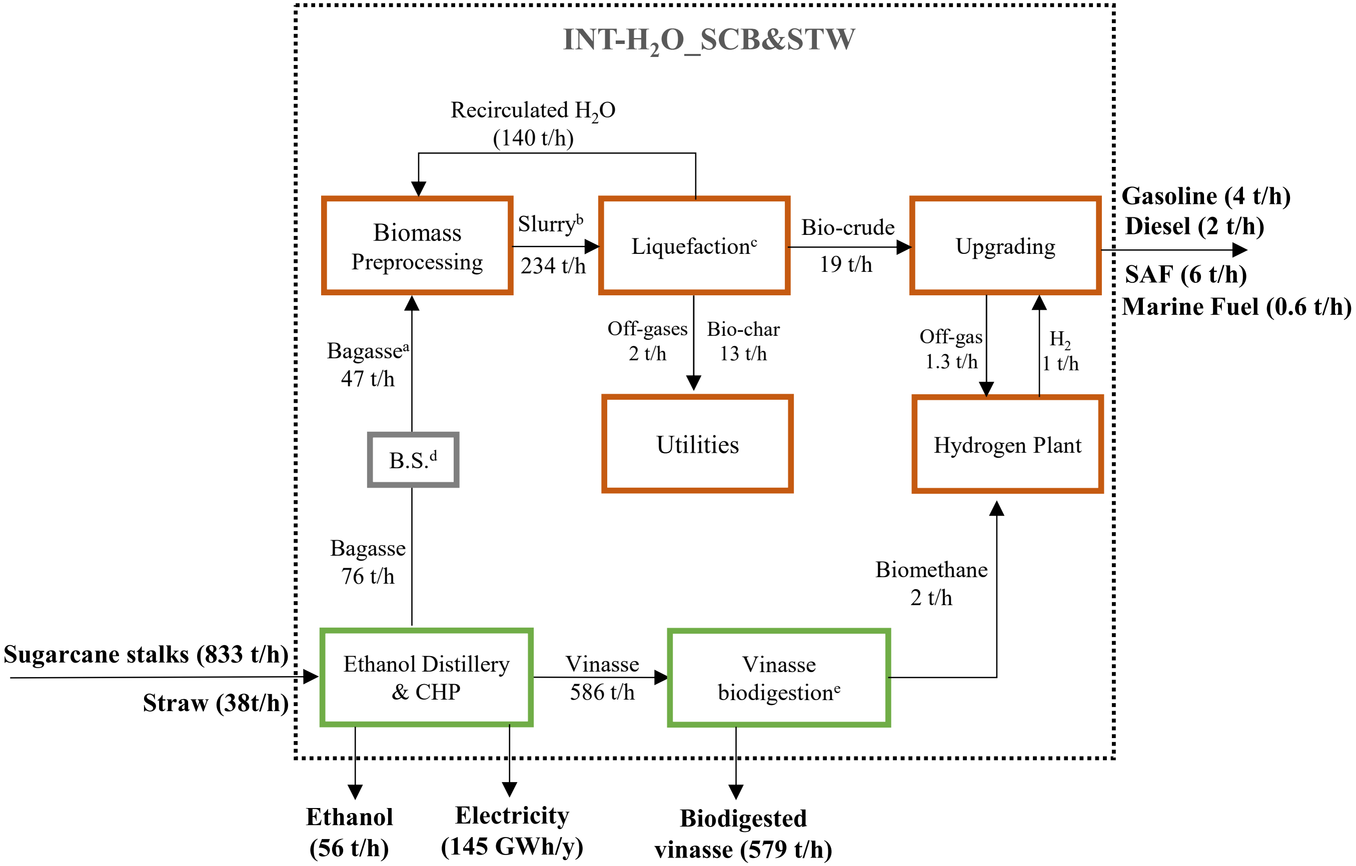

Figure S5. Mass fluxogram of INT-H_2O_SCB&STW

a: Bagasse mass given in dry basis.

b: The bagasse moisture was accounted for in the slurry.

c: Liquefaction and Products Separation.

d. Bagasse Storage.

e. Vinasse Biodigestion & Biomethane Upgrading

4. Techno-economic analysis

The Equation (S1) was used to scale and update the capital costs from the reference study [4].

$$\boldsymbol{CapEx_{2019}}(\boldsymbol{US}\$) = \boldsymbol{CapEx_{2007}}(\boldsymbol{US}\$)^{\mathbf{0,7}}.(\boldsymbol{Location\ Factor}).\left(\frac{\boldsymbol{CEPCI_{2019}}}{\boldsymbol{CEPCI_{2007}}}\right) \quad \text{Equation (S1)}$$

In order to calculate the production cost of the standard aviation fuel and the other products obtained in the biorefineries (both in stand-alone and integrated configurations) a cost allocation approach was adopted from the Virtual Biorefinery framework and from other studies [1,14,15]**. This cost allocation considered the share of each product on total revenue among the biorefinery products. Thus, all the operating and capital expenses were allocated according to the standard aviation fuel share on total revenues. For instance, if 40 % of the revenue comes from SAF,**

this proportion of 40% was maintained to allocate the expenses associated with sugarcane, bagasse, straw, chemical inputs, maintenance, wages, capital costs, and so on, to SAF.

Table S3. CAPEX of the stand-alone scenarios

Area Description, MUS$	**SA-EtOH_SCB**	**SA-H_2O_SCB**	**SA-H_2O_STW**
Area 1-Biomass Preprocessing	18	18	12
Area 2-Liquefaction/Product Recovery	65	65	65
Area 3-Hydrotreating	28	25	25
Area 4-Hydrogen Generation	17	17	17
Area 5- Utilities & Waste Water Treatment	18	15	15
Total Installed Cost, TIC	146	139	134
Total Direct Costs, TDC (14,5% of TIC)	21	20	19
Indirect costs (55% of TDC)	92	88	84
Fixed Capital Investment, FCI	259	247	237
Working capital (10% of FCI)	26	25	24
Total capital investment	285	272	261

Table S4. HTL CAPEX of the integrated scenarios

Area Description	**Scenario**	
ETHANOL DISTILLERY, MUS$	**INT-EtOH_SCB&STW**	**INT-H2O_SCB&STW**
Area 1- Sugarcane & Straw Preprocessing	15	15
Area 2-Juice Extraction	25	25

Area 3-Juice Treatment	17	17
Area 4- Juice Fermentation	17	17
Area 5- Ethanol Distillation	48	48
Area 6- Steam System & Power Generation	124	124
Area 7- Vinasse Biodigestion	41	41
Buildings, Auxiliaries	38	37
Fixed Capital Investment, 1G	**325**	**324**
HTL, MUS$		
Area 8-Feedstock Handling	18	18
Area 9-Liquefaction/Product Recovery	65	65
Area 10-Hydrotreating	28	25
Area 11-Hydrogen Generation	18	15
Total Installed Cost, TIC	129	123
Total Direct Costs, TDC (14,5% of TIC)	19	18
Indirect costs (55% of TDC)	81	77
Fixed Capital Investment, 2G	**229**	**218**
Total Fixed Capital Investment, FCI	554	542
Working capital (10% of FCI)	55	54
Total capital investment	**609**	**596**

5. Life cycle assessment

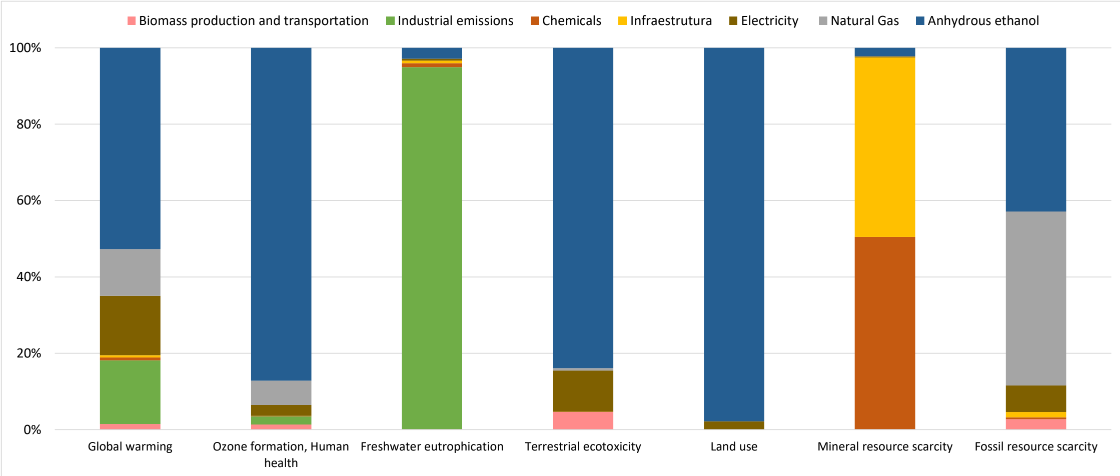

Figure S6. Environmental impact breakdown for the selected categories of SA-EtOH_SCB

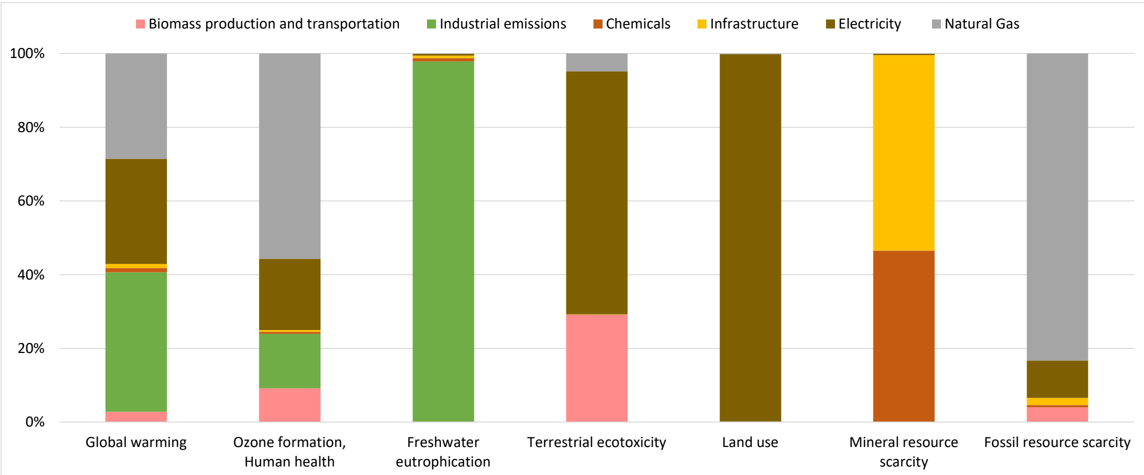

Figure S7. Environmental impact breakdown for the selected categories of SA-H_2O_SCB

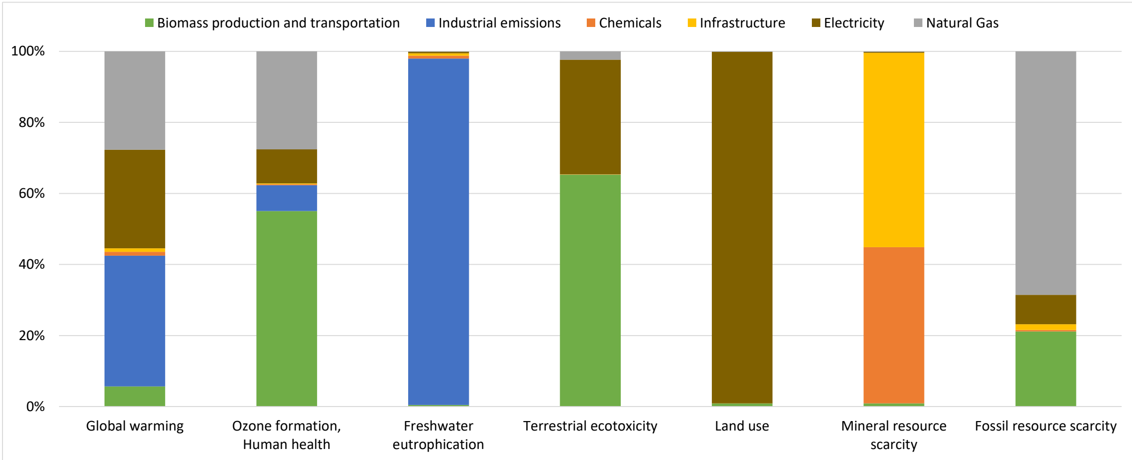

Figure S8. Environmental impact breakdown for the selected categories of SA-H_2O_SCB

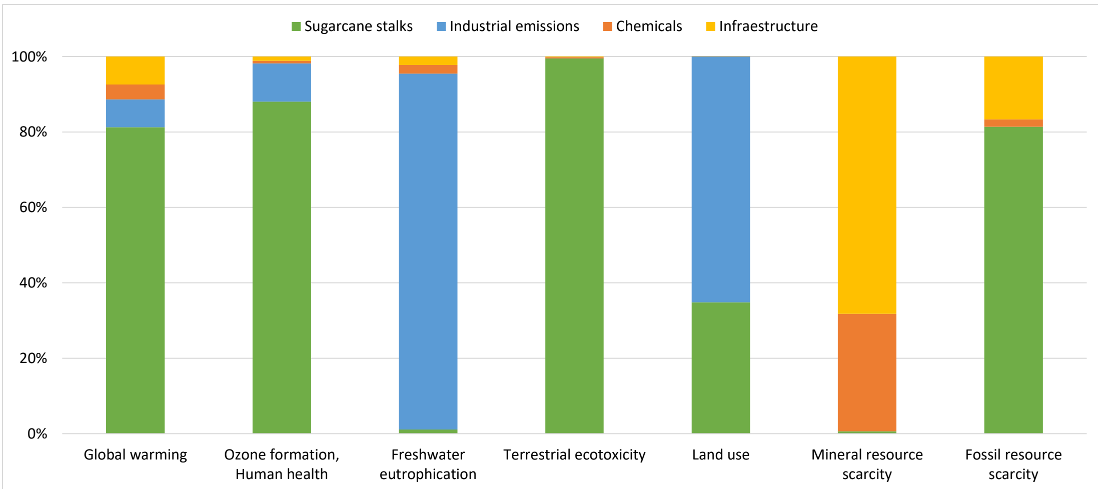

Figure S9. Environmental impact breakdown for the selected categories of INT-EtOH_SCB&STW

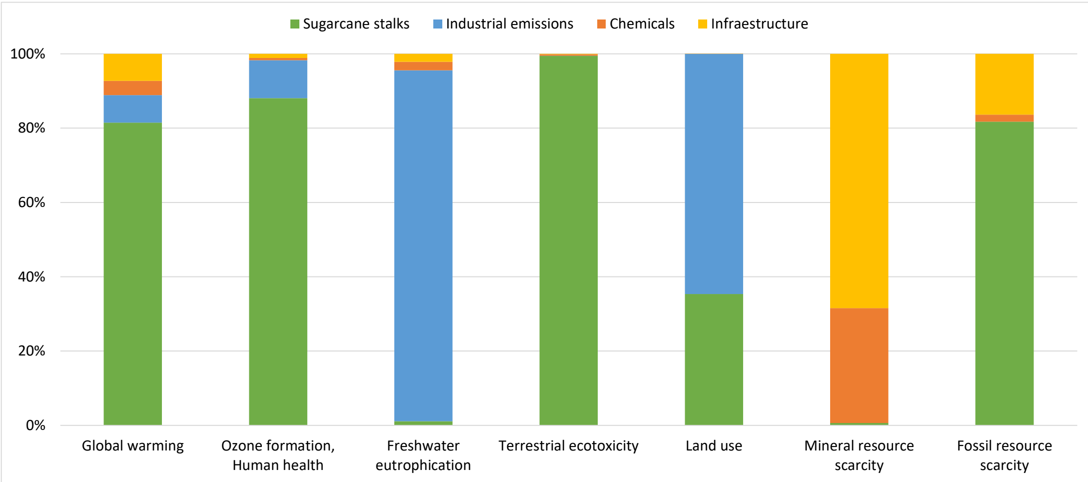

Figure S10. Environmental impact breakdown for the selected categories of INT-H_2O_SCB&STW

Table S5. Life Cycle Inventory of the evaluated scenarios

Flows	Unit/ year	SA-EtOH _SCB	SA-H2O _SCB	SA-H2O _STW	INT-EtOH_ SCB&STW	INT-H2O_ SCB&STW
Inputs						
Natural resources						
Air	t	1,223,730	1,186,192	1,186,192	2,659,262	2,659,262
Occupation, industrial area, built up	m2a	0.0042	0.0040	0.0039	0.03	0.03
Transformation, from agriculture	m2	0.0001	0.0001	0.0001	0.001	0.001
Transformation, to industrial area, built up	m2	0.0001	0.0001	0.0001	0.001	0.001
Materials/fuels						
Sugarcane	t	-	-	-	4,000,000	4,000,000
Sugarcane straw (wet)	t	-	-	436,553	183,400	183,400
Bagasse (wet)	t	742,140	742,140	-	-	-
Quicklime, milled, packed, at plant/CH U	t	-	-	-	2,550	2,550
Sulphuric acid, liquid, at plant, market mix/CTBE BR U	t	-	-	-	1,696	1,696
Phosphoric acid, industrial grade, 85% in H2O, at plant/RER U	t	-	-	-	875	875
Chemicals inorganic, at plant/GLO U	t	-	-	-	11	11
Chemicals inorganic, at plant/GLO U	t	-	-	-	4	4
Zeolite, powder, at plant/RER S	t	203	172	172	443	443
Water treatment biorefinery/CTBE BR U	m^3	409,122	215,167	40,459	4,410,353	4,215,814
Bagasse, to combustion/CTBE BR U	t	-	-	-	401,684	401,684
Bio-char, to combustion/CTBE BR U		84,679	85,878	85,878	-	-
Off-gases, to combustion/CTBE BR U	t	3,238	0	0	0	0
Lubricating oil, market mix/CTBE BR U	t	-	-	-	13	13
Steel product manufacturing, average metal working/RER U	t	337	322	309	5,379	5,268
Chromium steel product manufacturing, average metal working/RER U	t	20	19	18	314	307

Concrete, sole plate and foundation, at plant/CH U	m³	458	437	420	7,206	7,057
Building, hall, steel construction/CH/I U	m2	96	91	88	1,507	1,476
Electricity, high voltage, at grid/CTBE BR U	kwh	69,175	67,202	67,202	-	-
Natural gas, production BR, at long distance pipeline/CTBE BR U	m³	9,217	11,331	11,331	0	0
Anhydrous ethanol, Book2015, 1.2.2/CTBE BR U	t	111,462	-	-	-	-
Sodium hydroxide, without water, in 50% solution state {GLO}	t	-	-	-	162	162
Iron ore, beneficiated, 65% Fe {GLO}| market for | Cut-off, U	t	-	-	-	1.61	1.61
Triethylene glycol {RoW}|	t	-	-	-	0.13	0.13
Outputs						
Main products						
Sustainable aviation fuel	t	67,210	50,432	50,432	67,210	50,432
Green gasoline	t	40,326	30,259	30,259	40,326	30,259
Green diesel	t	20,163	15,129	15,129	20,163	15,129
Marine fuel	t	6,721	5,043	5,043	6,721	5,043
Anhydrous ethanol	t	0	0	0	159,780	271,241
Electricity	GWh	0.00	0.00	0.00	145	145
NVG (from biomethane)	MNm3	-	-	-	4	2
Sulphur	t	-	-	-	333	333
Residues sent to the field						
Vinasse (biodigested)	t	-	-	-	2,811,597	2,811,597
Filter cake (wet)	t	-	-	-	163,469	163,469
Ash (dry)	t	-	-	-	19,281	19,281
Soil (from sugarcane cleaning and boiler)	t	-	-	-	12,524	12,524
Emissions to air						
Carbon dioxide, biogenic	t	-	-	-	924,690	924,690
Methane, biogenic	t	-	-	-	22.01	22.01
Carbon dioxide, fossil	t	18,206	22,382	22,382	-	-
NMVOC	t	5.72	5.51	5.51	-	-
Methane, fossil	t	0.22	0.21	0.21	-	-
Carbon monoxide, fossil	t	4.46	4.30	4.30	-	-
Dinitrogen monoxide	t	0.14	0.13	0.13	-	-

Nitrogen oxides	t	11.19	10.77	10.77	-	-
Sox (sulfur dioxide)	t	0.06	0.05	0.05	0.01	0.01
PM (particulates, unspecified)	t	1.67	1.61	1.61	-	-

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