

Supplementary Material

Sustainable aviation fuel from forestry residue and hydrogen – a techno-economic and environmental analysis for an immediate deployment of the PBtL process in Europe

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Modelling Assumptions

Tab. 1. Modelling assumptions implemented in Aspen Plus®.

Unit	Description	Source
Dryer	Biomass moisture outlet: 15 wt-%, heat consumption: $1300 \text{ kWh/t}_{\text{H}_2\text{Oevap}}$, power consumption: $32 \text{ kWh/t}_{\text{drybio}}$, pressure: 1 bar	¹
Gasifier	Heat loss = 1 % of input biomass LHV. $\Delta p = -0.2 \text{ bar}$. $T = 850^\circ\text{C}$, $p = 4.0 \text{ bar}$ ¹ Oxygen feed iterated to attain specified heat loss Minimum CO_2/O input = 1.0 (mass based) Feeding temperature = 200°C Modelled with RStoic and RGibbs. RGibbs (PR-BM) temperature 900°C Hydrocarbon formation (mol/kg of fuel volatiles): $\text{CH}_4 = 6.7826$, $\text{C}_2\text{H}_4 = 0.4743$, $\text{C}_2\text{H}_6 = 0.2265$, $\text{C}_6\text{H}_6 = 0.2764$ Tars modelled as naphthalene: $\text{C}_{10}\text{H}_8 = 0.0671$ Fuel nitrogen converted to NH_3 Fuel sulphur converted to H_2S Fuel ash to 100% to fly ash Fuel carbon: 0.05 % to fly ash All other components assumed to be in simultaneous phase and chemical equilibrium.	
Filter	$\Delta p = -0.2 \text{ bar}$. Inlet temperature 550°C Complete removal of ash	¹
Reformer	$T = 850^\circ\text{C}$ Adiabatic Oxygen feed iterated to attain specified heat loss Modelled as RGibbs Phase and chemical equilibrium conversion for C_{2+} and tar. CH_4 conversion: 35 % NH_3 conversion: 50 % $\Delta p = -0.2 \text{ bar}$	¹
Water scrubber	Scrubbing liquid: water. $T_{\text{inlet}} = 200^\circ\text{C}$. Two-step cooling: $T_{1 \text{ out}} = 60^\circ\text{C}$, $T_{2 \text{ out}} = 30^\circ\text{C}$. Modelled as Flash using Soave-Redlich-Kwong (SRK) equation of state model.	¹
Syngas compressor	$p_{\text{out}} = 25 \text{ bar}$ 5 stages with intercooling to 100°C Equal pressure ratio Isentropic efficiency 80 % Mechanical efficiency 100 %	¹

Selexol scrubber	T = 0 °C 90 % removal of CO ₂ removal of ammonia (100%) and H ₂ S (90 %) Modelled as a separator block Energy consumption: 74 kJ/kg _{CO₂,removed} CO ₂ outlet pressure: 1 bar	2, 3
Guard bed	Complete removal of trace components Modelled as a separator block	4
FT reactor	220 °C, 25 bar, Slurry bubble column reactor Catalyst mass iterated to reach 55 % CO conversion Kinetic reaction model from ⁵ Products: n-alkanes and primary alkenes with a carbon chain length up to 30	5
Product separation	Tout = 0 °C Modelled with separator blocks Complete separation of Products C ₅₊ Recycle ratio 95 % of tail gas	
AEL	70.8 % HHV efficiency Modelled as a splitter p = 25 bar Hydrogen output iterated for a H ₂ /CO = 2.1 at FT inlet	6
CO ₂ Compressor	One stage compression Isentropic efficiency: 80 % Mechanical efficiency: 100 %	1

Tab. 2. FCI factors for equipment cost estimation methods.

Indirect cost factors	1	2	3	4	5
Source	7	8	1	1	
Installation factor	0.39	0.1	0	0	0
Instrumentation and control	0.26	0.36	0	0	0
Piping system	0.31	0.5	0	0	0
Electrical systems	0.1	0.1	0	0	0
Buildings	0.29	0.18	0	0	0
Yard improvements	0.12	0.1	0	0	0
Service facilities	0.55	0.4	0	0	0
Engineering and supervision	0.32	0.32	0.15	0.10	0

Construction cost	0.34	0.41	0	0	0
Legal expenditure	0.04	0.04	0	0	0
Contractor's fee	0.05	0.05	0	0	0
Contingency	0.1	0.1	0	0	0

Tab. 3. Indirect operating expenditure factors taken from [46].

	Factor [%]	Basis
Operating supervision (OS)	15	OL
Maintenance labour (ML)	1	FCI
Maintenance material (MM)	1	FCI
Operating supplies	15	ML + MM
Laboratory charges	20	OL
Insurances and taxes	2	FCI
Plant overhead costs (PO)	60	Total labour cost (OL + OS + ML)
Administrative costs	25	PO
Distribution and selling cost	6	NPC
Research and development costs	4	NPC

Mass balances

The stream data for selected process streams is presented in Tab. 4. The streams are numbered according to the order shown in Fig. 1.

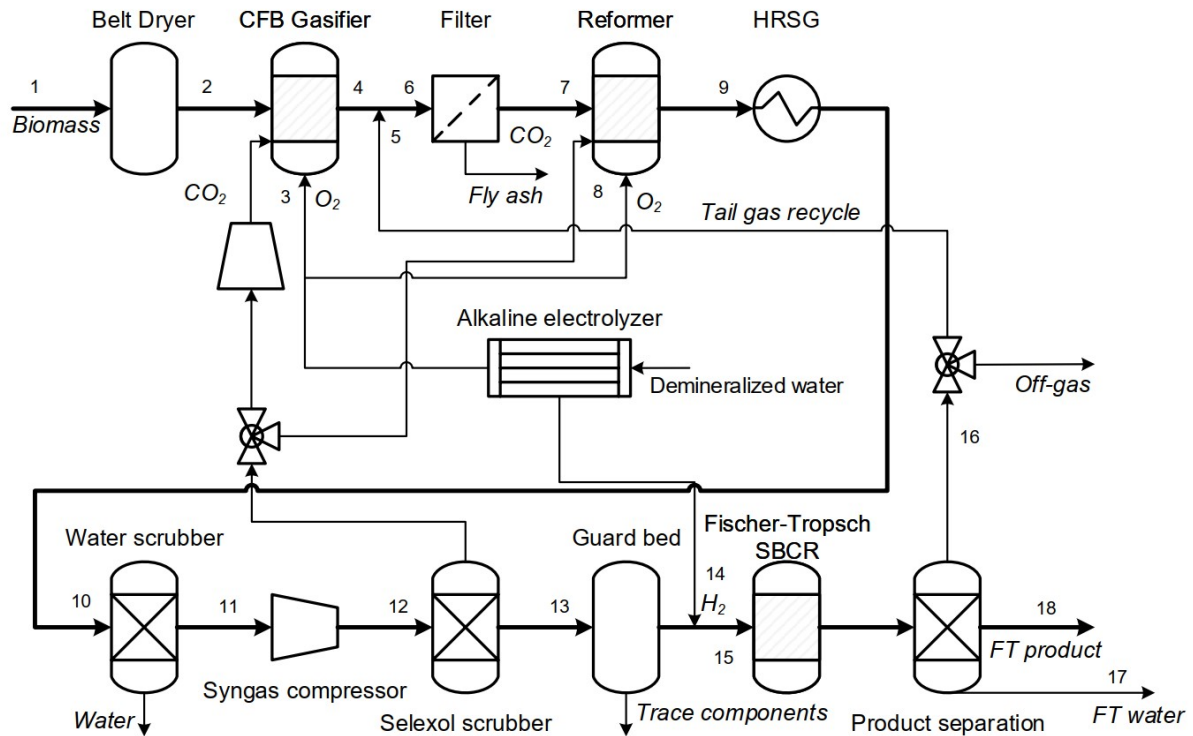


Fig. 1. Process flowsheet with stream numbers as referred to in Tab. 4.

Tab. 4. Stream data for selected process streams.

Stream number	1	2	3	4	5	6
	Wet biomass feed Dryer	Gasifier feed	Recycle and oxygen to Gasifier	Syngas from Gasifier	Recycle syngas	Filter feed
Temperature °C	25.0	65.5	199.9	850.0	0.0	600.0
Pressure bar	1	1	4	3.8	24.9	3.8
Molar flow kmol/s			0.4946	1.8158	3.2024	5.0182
Mass flow kg/s	47.3569	27.857	18.3523	46.2093	40.3801	86.5894
Composition						
H2	mol/mol			0.1901	0.5451	0.4167
CO	mol/mol			0.3561	0.2831	0.3095
CO2	mol/mol		0.425	0.2399	0.0173	0.0979
H2O	mol/mol			0.1386		0.0502
O2	mol/mol		0.575			
N2	mol/mol				0.0075	0.0048
CH4	mol/mol			0.0626	0.1383	0.1109
C2H6	mol/mol			0.0021	0.0016	0.0018
C3H8	mol/mol				0.0014	0.0009

C4H10	mol/mol			0.0013	0.0008
C10H8	mol/mol				0.0002
C6H6	mol/mol				0.0009
NH3	mol/mol		0.0006		0.001
H2S	mol/mol		0.0026		0.0001
C2H4	mol/mol			0.0002	0.0017
C3H6	mol/mol		0.0028	0.0025	0.0016
C4H8	mol/mol		0.0002	0.0017	0.0011
Other components					
Biomass	kg/s	47.3569	27.857		
Fly ash	kg/s			0.9298	0.9298

Stream number		7	8	9	10	11
		Reformer feed	CO2 recycle and oxygen to Reformer	Syngas to HRSG	Syngas to Water Scrubber	Syngas to Compressor
Temperature	°C	600.0	199.8	900.0	60.0	30
Pressure	bar	3.6	3.6	3.4	3.4	3.4
Molar flow	kmol/s	5.0182	0.6217	5.9766	5.9764	5.2841
Mass flow	kg/s	85.6596	23.6827	109.3423	109.3415	96.869

Composition

H2	mol/mol	0.4167		0.3581	0.3581	0.405
CO	mol/mol	0.3095		0.3547	0.3547	0.4012
CO2	mol/mol	0.0979	0.5072	0.0977	0.0977	0.1105
H2O	mol/mol	0.0502		0.1242	0.1242	0.0095
O2	mol/mol		0.4928	0.	0.	
N2	mol/mol	0.0048		0.0042	0.0042	0.0048
CH4	mol/mol	0.1109		0.0605	0.0605	0.0685
C2H6	mol/mol	0.0018				
C3H8	mol/mol	0.0009				
C4H10	mol/mol	0.0008				
C10H8	mol/mol	0.0002				

C6H6	mol/mol	0.0009				
NH3	mol/mol	0.001		0.0004	0.0004	0.0005
H2S	mol/mol	0.0001		0.	0.	0.0001
C2H4	mol/mol	0.0017				
C3H6	mol/mol	0.0016				
C4H8	mol/mol	0.0011				

Stream number		12	13	14	15	16	17
		Syngas to Selexol Scrubber	Syngas to Guard Beds	Hydrogen from Electrolyzer	Syngas to Fischer-Tropsch Reactor	Fischer-Tropsch gas fraction	FT Water
Temperature	°C	0	0	60	220	0	25
Pressure	bar	25	25	25	25	24.9	24.9
Molar flow	kmol/s	5.2841	4.7055	2.2061	6.9115	3.3709	1.1658
Mass flow	kg/s	96.869	72.7807	4.4472	77.2269	42.5053	21.0028
Composition							
H2	mol/mol	0.405	0.4548	1.	0.6288	0.5451	
CO	mol/mol	0.4012	0.4505		0.3067	0.2831	
CO2	mol/mol	0.1105	0.0124		0.0084	0.0173	
H2O	mol/mol	0.0095					1.
O2	mol/mol						
N2	mol/mol	0.0048	0.0054		0.0037	0.0075	
CH4	mol/mol	0.0685	0.0769		0.0523	0.1383	
C2H6	mol/mol					0.0016	
C3H8	mol/mol					0.0014	
C4H10	mol/mol					0.0013	
C10H8	mol/mol						
C6H6	mol/mol						
NH3	mol/mol	0.0005					
H2S	mol/mol	0.0001	0.				
C2H4	mol/mol					0.0002	

Tab. 5. Utility cost and revenue form by-products.

Utility/Raw material	Quantity per hour	Market price (2020)	Total costs per year [€/a]	
Electricity	943.6(MWh)	50.4(€/MWh)	385201017.2	
Cooling Water	38535.1(m ³)	0.005(€/m ³)	1560670.61	
Biomass	170.5(t)	42.232(€/t)	58,319,311	
Demineralized water	153.9(m ³)	2.032(€/m ³)	2,533,575	
Cobalt catalyst	7.9(kg)	32.918(€/kg)	2,094,963	
Selexol	0.0034(t)	4394.808(€/t)	121,389	
Stack maintenance	16010.0(kg)	0.109(€/kg)	14,135,217	
Waste Water	126.5(m ³)	0.918(€/m ³)	1,059,734	
Total costs:			465,339,078	
By-products	Quantity per hour	Market price (2020)	Total revenue per year [€/a]	
Low Pressure Steam	-319.95(t)	13.142(€/t)	-	34,058,741
Medium Pressure Steam	-109.3392(t)	16.057(€/t)	-	14,220,842
High pressure steam	-195.8112(t)	17.706(€/t)	-	28,082,968
Total revenue:			-	76,362,552

Tab. 6. Equipment cost and fixed capital investment cost for all process units.

	Equipment cost [M€]	Fixed capital investment [M€]
Dryer	37.64	37.64
AEL Stack	686.43	686.43
AEL BoP	60.87	247.12
Filter	19.52	29.18
Guard Bed	31.74	38.41

Selexol	24.24	103.70
Striper	16.94	24.12
CFB gasifier	58.78	71.13
HRS	20.32	30.37
Refrigeration System	6.97	29.81
CO ₂ Compressor	2.42	3.45
Syngas Compressor	16.37	23.32
Reformer	50.20	71.50
FT SBCR Vessel	13.99	59.85
FT SBCR Catalyst	18.14	77.59
Cold Trap	0.09	0.38
Total	1,064.66	1,534.00

Tab. 7. Annuity calculation.

Fixed Capital Investment [FCI]	1,534.00	M€
Working capital	10.00%	of TCI
Total Capital Investment [TCI]	1,704.44	M€
Operating time of plant	20	years
Interest rate	7.00%	
Annuity factor	0.094392926	
Annuity	156.73	M€/year

Tab. 8. Net production cost calculation (NPC).

Direct production costs	Cost per year [M€/a]
Operating labour [OL]	3.45
Operating supervision	0.52
Maintenance labour	15.34

Maintenance material	15.34
Operating supplies	4.60
Laboratory charges	0.69
Raw materials and utilities	464.91
Revenue from by-products	- 76.36
Indirect production costs	-
Insurances and taxes	30.68
Plant overhead costs	11.59
General expenses	-
Administrative costs	2.90
Annuity	156.73
	630.38
Indirect production costs	Cost per year [M€/a]
Distribution and selling costs	42.03
Research and development costs	28.02
Production cost	700.42
Product output per year [Mt/a]	0.40
Net production cost [€/kg]	1.75

Local economic/ecologic analysis

Tab. 9. National economic/ecologic conditions relevant for the PBtL production.

NUTS0	Electricity price [€/MWh] ⁹	Carbon intensity [gCO₂eq/kWh] ¹⁰	Labour cost [€/h] ¹¹	Transport Cost [€/t/km] ¹²
FR	53.5	51.1	37.5	0.48
AL	51.6	-	2.6 ^a	0.18
AT	73.6	82.4	36.7	0.45
BA	62.7	-	5.2 ^a	0.19
BE	41.8	161.0	41.1	0.47
BG	57.9	410.4	6.5	0.22
CY	114 ^a	620.9	17	0.36
CZ	63.2 ^a	436.6	14.1	0.29
DE	64.3	311.0	36.6	0.45
DK	47.1	109.0	45.8	0.68
EE	68.8 ^a	774.9	13.6	0.28

EL	59.7 ^a	479.2	16.9	0.37
ES	50.3	156.4	22.8	0.41
FI	45.9	68.6	34.3	0.49
HR	58.4	133.8	10.8	0.26
HU	65.6	216.4	9.9	0.24
IE	78.6	278.6	32.3	0.44
IT	57.8	213.4	29.8	0.45
LT	63.2 ^a	45.4	10.1	0.24
LU	47.3 ^a	58.5	42.1	0.48
LV	69.5 ^a	106.5	10.5	0.26
ME	56.9	-	5.6 ^a	0.2
MK	53.4	-	3.6 ^a	0.17
MT	86 ^a	379.0	14.5	0.3
NL	59.5	328.4	36.8	0.5
NO	30.8	19 ^d	47.3	0.53 ^c
PL	75.3	709.8	11	0.27
PT	69.8	198.4	15.7	0.29
RO	67.5	299.5	8.1	0.21
RS	58.3	-	5.8 ^a	0.19
SE	35.6	8.8	37.3	0.53
SI	65.2 ^a	217.8	19.9	0.32
SK	94.4	101.7	13.4	0.27
UK	136.1	225.0	28.5 ^a	0.48

a data from past years used instead of 2020S1.

b Electricity price from 70 – 150 GWh consumer category.

c Assumed same transport cost as Sweden

d Value from 2019 used ¹³

GHG Abatement cost calculation

Tab. 10. Assumptions for the GHG abatement calculation.

	<i>Value</i>	<i>Unit</i>
Oil price (Brent)¹⁴	75.06	\$/barrel
Volumetric conversion¹³	158.98	l/barrel
Currency conversion¹⁵	0.877	€/€
Oil price	0.415	€/l

Impact categories for LCA

Tab. 11. Impact categories used in the LCA.

Impact category	Indicator	Unit	Abbreviation
Climate change	Radiative forcing as Global Warming Potential (GWP100)	kg CO ₂ eq	GWP
Ozone depletion	Ozone Depletion Potential (ODP)	kg CFC-11eq	ODP
Particulate matter/ Respiratory inorganics	Human health effects associated with exposure to PM2.5	Disease incidences	PM
Photochemical ozone formation	Tropospheric ozone concentration increase	kg NMVOC eq	POF
Acidification	Accumulated Exceedance (AE)	mol H+ eq	AP
Eutrophication, terrestrial	Accumulated Exceedance (AE)	mol N eq	TEP
Eutrophication, aquatic freshwater	Fraction of nutrients reaching freshwater end compartment (P)	kg P eq	FEP
Eutrophication, aquatic marine	Fraction of nutrients reaching marine end compartment (N)	kg N eq	MEP
Ecotoxicity (freshwater)	Comparative Toxic Unit for ecosystems (CTUe)	CTUe	FETP
Land use	Soil quality index (Biotic production, Erosion resistance, Mechanical filtration and Groundwater replenishment)	Dimensionless , aggregated index	LU
Water scarcity	User deprivation potential (deprivation-weighted water consumption)	kg world eq. deprived	WS
Resource use, minerals and metals	Abiotic resource depletion (ADP ultimate reserves)	kg Sb eq	MM
Resource use, energy carriers	Abiotic resource depletion – fossil fuels (ADP-fossil)	MJ	ECF

Economic allocation

Tab. 12. Economic allocation factors for the LCA.

Flow	Quantity [t/h]	Price [€/t]	Revenue [€/h]	Allocation factor
FT product	49.39	1,750.00	86,428.27	0.9016
Low Pressure Steam	319.95	13.14	4,204.78	0.0439
Medium Pressure Steam	109.34	16.06	1,755.66	0.0183
High pressure steam	195.81	17.71	3,467.03	0.0362
Total	-	-	95,855.74	1

Life Cycle Inventories

The following tables contain the data used to model the PBtL processes as part of the LCA. The names and locations of the process flows correspond to the ones used in the ecoinvent v3.7.1 database. In the processes that include electricity as an input (i.e. Selexol production and PBtL production) the electricity entry was adapted to correspond to the respective scenario (e.g. Swedish grid). For the sake of simplicity only one such case is shown here. The amounts shown here correspond to the base case as described in Section 6. Flows with no entry in the column “Location” are biosphere flows. Tab. 13 to Tab. 21 list the LCIs for the processes that make up the LCI of the entire PBtL production process shown in Fig. 1.

Tab. 13. LCI of the production of 1 kg of Selexol taken from ¹⁶.

Selexol production flows	Amount	Unit	Location
market for ethylene oxide	7.50E-01	kg	RER
market for methanol	0.2	kg	GLO
market for water, decarbonised	0.05	kg	DE
market for natural gas, high pressure	0.05	cubic meter	DE
steam production, in chemical industry	0.5	kg	RER
market for electricity, medium voltage	3.00E-01	kilowatt hour	EE
Water, cooling, unspecified natural origin	2.50E-02	cubic meter	
Methanol	1.00E-04	kg	
Ethylene oxide	1.00E-04	kg	

Tab. 14. LCI for the production of 1 kg of cobalt catalyst based on ⁵.

Cobalt catalyst production flows	Amount	Unit	Location
market for cobalt	0.25	kg	GLO
market for molybdenum	0.0356	kg	GLO
market for aluminium oxide, non-metallurgical	0.7452	kg	IAI Area, EU27 & EFTA
market for process-specific burdens, residual material landfill	1	kg	Europe without Switzerland

Tab. 15. LCI for the production of 1 kg of nickel catalyst based on the data acquired in the FLEXCHX project.

Nickel catalyst production flows	Amount	Unit	Location
market for nickel, class 1	0.15	kg	GLO
market for aluminium oxide, non-metallurgical	0.85	kg	IAI Area, EU27 & EFTA
market for process-specific burdens, residual material landfill	1	kg	Europe without Switzerland

Tab. 16. LCI for the production of 1 kg of guard bed material.

Guard bed material production flows	Amount	Unit	Location
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market for activated carbon, granular	1	kg	GLO
market for process-specific burdens, residual material landfill	1	kg	Europe without Switzerland

Tab. 17. LCI for the provision of 1 kg of forest residue biomass. This inventory is based in the ecoinvent activity "market for wood chips, wet, measured as dry mass, Europe without Switzerland", but adapted to not include the biomass coming from sawmills, in order to only describe primary residues. The transport activities contained in the original ecoinvent process were omitted here and explicitly included in the PBtL-production LCI as a separate flow.

Forest residue biomass flows	Amount	Unit	Location
hardwood forestry, birch, sustainable forest management	0.399	kg	SE
softwood forestry, spruce, sustainable forest management	0.1709	kg	SE
softwood forestry, pine, sustainable forest management	0.157	kg	SE
hardwood forestry, beech, sustainable forest management	0.137	kg	DE
softwood forestry, spruce, sustainable forest management	0.068	kg	DE
softwood forestry, pine, sustainable forest management	0.042	kg	DE
hardwood forestry, oak, sustainable forest management	0.027	kg	DE

Tab. 18. LCI for the construction of a PBtL plant corresponding to the base case of a 400 MW plant. The assumed lifetime is 20 years. This is a combination of data from ecoinvent processes for a syngas plant and a refinery plant each scaled to the capacity of the PBtL plant, and data from literature for the electrolysis plant (also scaled up to the modelled electrolyzer capacity) ¹⁷. The output of this process is one unit of PBtL plant.

PBtL plant construction flows	Amount	Unit	Location
synthetic gas factory construction	1.00E+02	unit	CH
petroleum refinery construction	4.00E-01	unit	RER
market for steel, low-alloyed	2.82E+07	kg	GLO
market for aluminium, cast alloy	7.04E+04	kg	GLO
market for chromium	1.53E+05	kg	GLO
market for nickel, class 1	3.13E+05	kg	GLO
market for polyethylene, high density, granulate	5.54E+04	kg	GLO

Tab. 19. LCI of the emissions and associated waste treatment processes from the production of 1 MJ of FT product as derived from the Aspen Plus model. The output of this process is one unit of emissions.

Emission flows	Amount	Unit	Location
market for wood ash mixture, pure	-1.54E-03	kg	Europe without Switzerland
Hydrogen (to air)	2.20E-09	kg	
Carbon monoxide, from soil or biomass stock (to air)	8.89E-09	kg	
Carbon dioxide, from soil or biomass stock (to air)	5.74E-03	kg	
Nitrogen (to water)	1.024E-10	kg	
Nitrogen (to air)	5.887E-05	kg	

Methane, from soil or biomass stock (to air)	6.06E-09	kg
Ammonia (to air)	7.168E-05	kg
Hydrogen sulfide (to water)	1.671E-05	kg

Tab. 20. LCI of other commodities needed for the production of 1 MJ of FT product as derived from the Aspen Plus model. The output of this process is one unit of other commodities.

Other commodity flows	Amount	Unit	Location
market for water, deionised	7.10E-02	kg	Europe without Switzerland
market for potassium hydroxide	1.48E-05	kg	GLO
Water, cooling, unspecified natural origin	1.78E-02	cubic meter	

Tab. 21. LCI of the modelled PBtL plant for the production of 1 MJ of FT product. The LCI includes the flows as listed in the tables above. Amounts in this LCI have been scaled with the economic allocation factor as presented in section 6.5.

PBtL production flows	Amount	Unit	Location
Forest residue biomass	4.17E-02	kg	Europe without Switzerland
transport, freight, lorry 16-32 metric ton, EURO6	7.09E-03	ton kilometer	RER
market for electricity, medium voltage	3.92E-01	kilowatt hour	SE
Other commodities	9.02E-01	unit	GLO
Selexol production	1.42E-06	kg	RER
Cobalt catalyst production	3.27E-06	kg	RER
Nickel catalyst production	2.74E-06	kg	RER
Guard bed material production	2.00E-06	kg	RER
Emissions	9.02E-01	unit	GLO
PBtL plant construction	2.566E-12	unit	RER

Additional visualisations

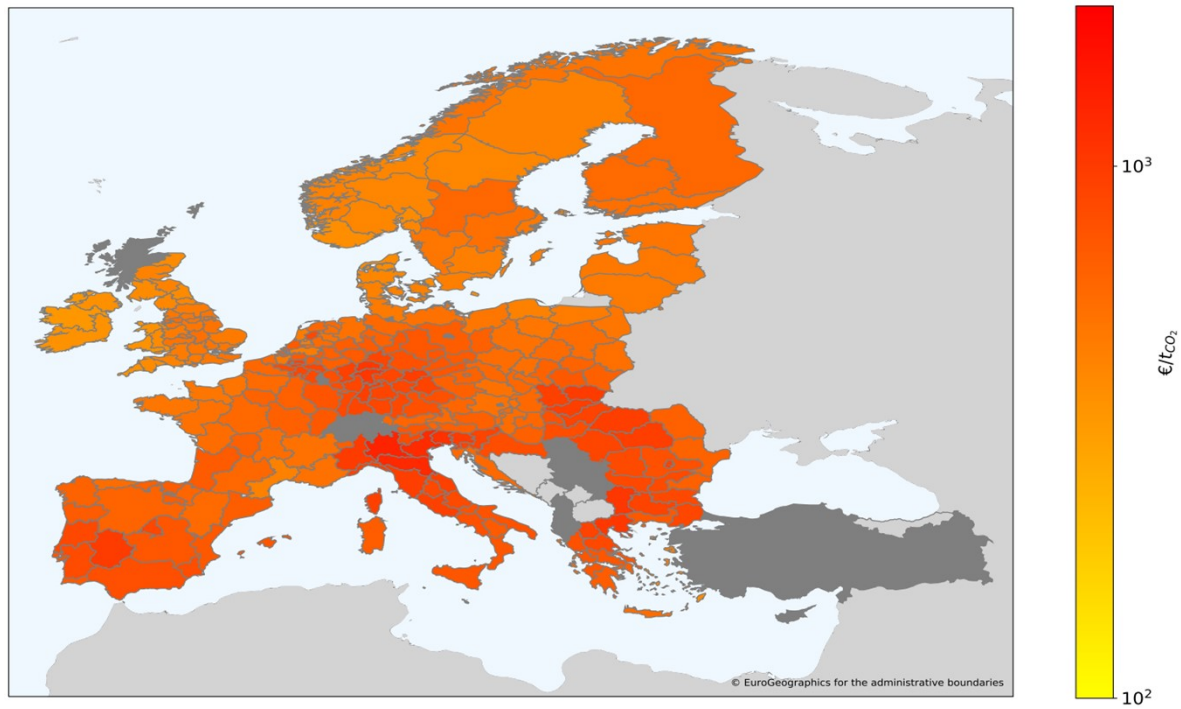


Fig. 2. Abatement cost [$\text{€}_{2020}/\text{t}_{\text{CO}_2}$] for wind park connected PBtL production in the hydrogen storage scenario.

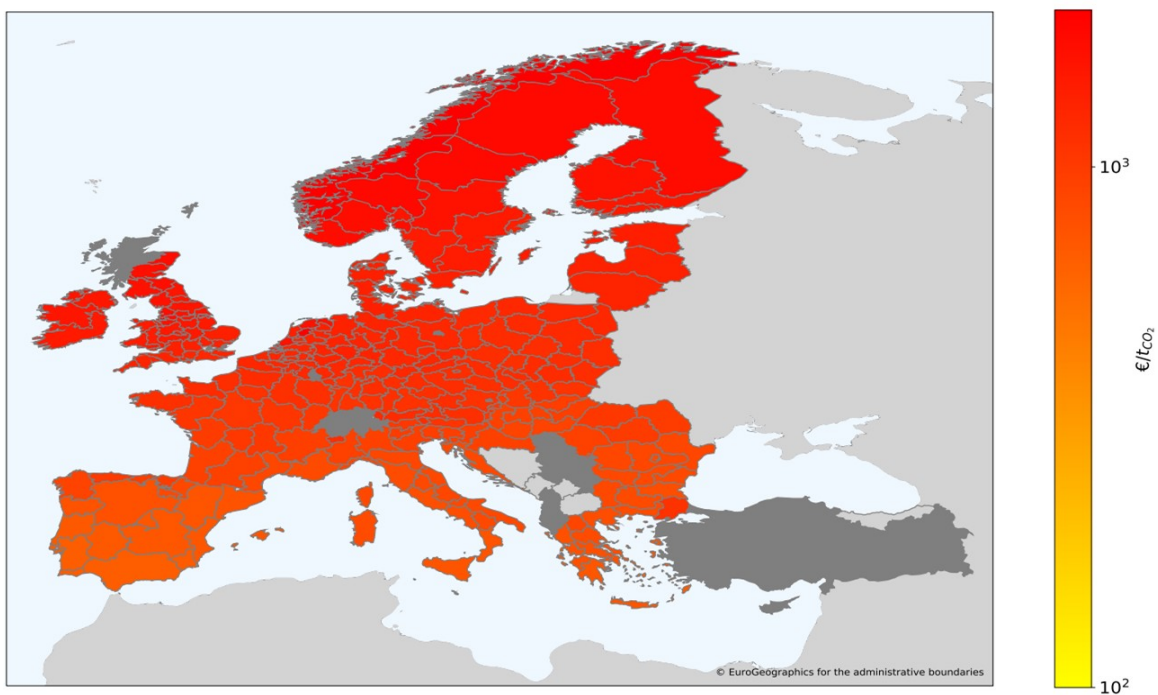


Fig. 3. Abatement cost [$\text{€}_{2020}/\text{t}_{\text{CO}_2}$] for PV connected PBtL production in 2020 in the hydrogen storage scenario.

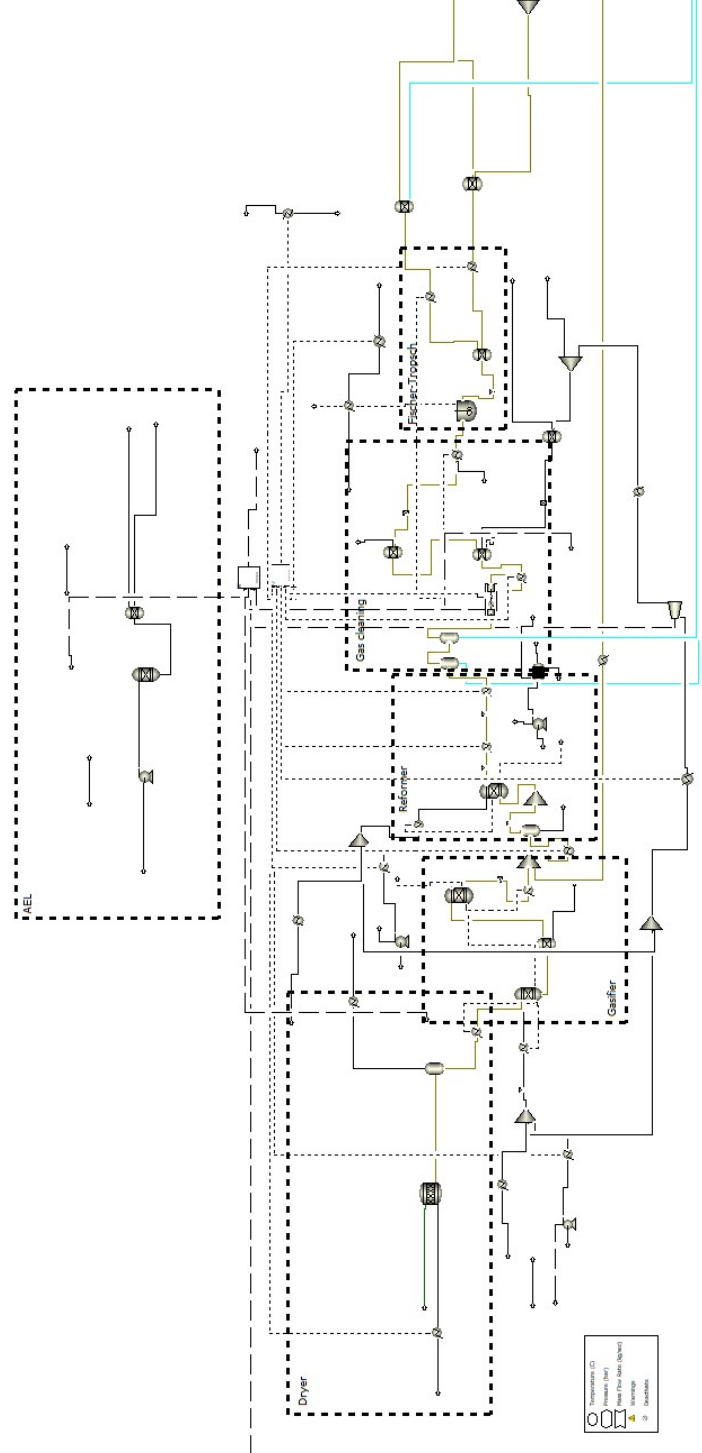


Fig. 4 Aspen Plus flowsheet of the PBtL process

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