Electronic Supporting Information (ESI)

Techno-economic feasible and sustainable C-lignin biorefinery

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List of abbreviations

• Aspen Capital Cost Estimator	ACCE
• Capital Expenditure	CAPEX
• Chemical Engineering's Plant Cost Index	CEPCI
• Combined Heat and Power	CHP
• Cash Flow Rate Of Return Analysis	DCFROR
• Ozone formation-Terrestrial ecosystems	EOFP
• Freshwater eutrophication	FEP
• Freshwater ecotoxicity	FETP
• Fossil resource scarcity	FFP
• Global warming potential	GWP
• Higher heating value	HHV
• Ozone formation-Human health	HOFP
• Human carcinogenic toxicity	HTPc
• Human non-carcinogenic toxicity	HTPnc
• Ionizing radiation	IRP
• Life cycle assessment	LCA
• Life cycle inventory	LCI
• Life cycle impact assessment	LCIA
• Land use	LOP
• Marine eutrophication	MEP
• Marine ecotoxicity	METP
• Minimum selling price	MSP
• National Renewable Energy Laboratory	NREL
• Net present value	NPV
• Stratospheric ozone depletion	ODP
• Operating expenses	OPEX
• Polyhydroxyalkanoates	PHA
• Fine particulate matter formation	PMFP
• 4-(3-Hydroxypropyl)benzene-1,2-diol (CAS: 46118-02-9)	Propanolcatechol
• 4-Propylcatechol (CAS: 2525-02-2)	Propylcatechol
• Pressure swing adsorption	PSA
• Reductive catalytic fractionation	RCF
• Mineral resource scarcity	SOP
• Terrestrial acidification	TAP
• Tertbutyl catechol	TBC
• Techno-economic analysis	TEA
• Terrestrial ecotoxicity	TETP
• Total installed capital cost	TIC
• Water consumption	WCP

Determination of minimum selling price

$$\text{NPV} = \sum_{t=1}^{n} \frac{C_t}{(1+r)^t} - C_0$$

Where r is discount rate, C_t is the net cash flow at time t, C_0 is initial investment. The minimum selling price is determined by iteratively adjusting the selling cost of catechol until the net present value of the project reaches zero.

C_t = Total annual sales (t) - Loan interest payment (t) - Total product cost (t) - Depreciation charge (t)

C_0 = Cumulative Investments + Interest

The calculation details are documented in Excel files.

Process description and modelling details

Table S1 Full biomass compositions

Castor seed coat definition	Reference
Cellulose	Native Aspen component (dextrose)
hemicellulose	Native Aspen component (d-xylose)
Available C-lignin	Native Aspen component (vanillin)
Other components	Native Aspen component (vanillin)
Extractives	Native Aspen component (dextrose)
ash	Native Aspen component CaO
Moisture	Native Aspen component H_2O
C-lignin intermediates	Solubilized C-lignin and extractives

The pumps, compressors, heat exchangers and flash drums are modeled using the default models embedded in Aspen Plus® V12. RADFRAC model is chosen for distillation columns modeling. The pretreatment reactor in A100 is modeled using RStoic model. Hydrogenolysis reactor in A200 and dealkylation reactor in A400 are modeled using RYield reactor due to the complexity of reactions. [1]

Non-random two-liquid (NRTL) model is set as the default thermodynamic model for this simulation given the non-ideality of the components used in the simulation. Since the hydrogenolysis reaction occurs in a polar system and under high pressure (>10 bar), the PSRK EOS is selected as the property method for simulating the hydrogenolysis area (A200).

The thermodynamic and physical properties of pure component are retrieved from native aspen database or estimated using the National Institute of Science and Technology ThermoDataEngine (NIST-TDE) capabilities built into the Aspen Plus software. Binary interaction parameters were estimated using UNIFAC.

Area 100 (A100): **Pretreatment.** In this area, castor seed coats are extracted using methanol at a mass ratio of 1:4.4 (feedstock to methanol) and 70 °C under 1.3-1.5 bar. After pretreatment, the obtained slurry is filter separated and the liquid fraction is sent to A200 after the partial methanol recovery whilst the solid fraction is sold as the co-product pulp.

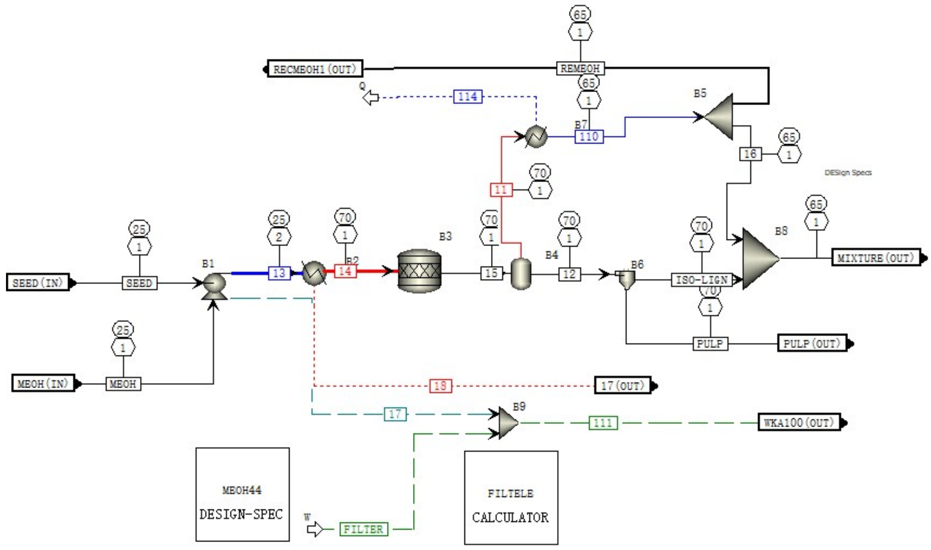


Fig. S1 Aspen Plus simulation flowchart for Pretreatment (A100) section

Area 200 (A200): Catalytic Hydrogenolysis. The reductive depolymerization occurs in a semi-continuous system using four parallel batch hydrogenation autoclaves, each operating in a staggered configuration. This allows three reactors to run simultaneously while one undergoes loading or unloading. The reductive depolymerization operated at the mass ratio of C-lignin intermediates to methanol of 0.23 and yield lignin oil consists of propanolcatechol, propylcatechol, and catechol oligomers and trace of methane generated via the hydrogenolysis of methanol. [2] Before heating the reactor to 200°C, the hydrogenolysis reactor is sealed, purged with nitrogen, and then pressurized with H_2 (3 MPa) in the presence of the 5 wt% Ru/C catalyst (catalyst to C-lignin sample). After the catalytic hydrogenolysis, the mixture stream is sent through a series of flash tanks to remove non-condensable vapors such as H_2, CH_4, CO_2, CO and recover methanol by the vapor fraction condensation. The reaction slurry (unreacted solids) is cooled down to suppress chemical reaction, depressurized, and filtered by filter pressing. Pressure swing adsorption is capable of separating ultra-pure hydrogen (with a purity of over 99.99%) from various gas mixtures and has become one of the most widely applied hydrogen purification technologies globally.[3] In scenario analysis, the gaseous fraction is sent to PSA unit to recover unreacted H_2 and methanol for recycling back to the reactors. The efficiency of hydrogen recycling can reach 85%. After the hydrogenolysis, the obtained stream is centrifuged to separate unreacted solid from the C-lignin oil which is sent to A300.

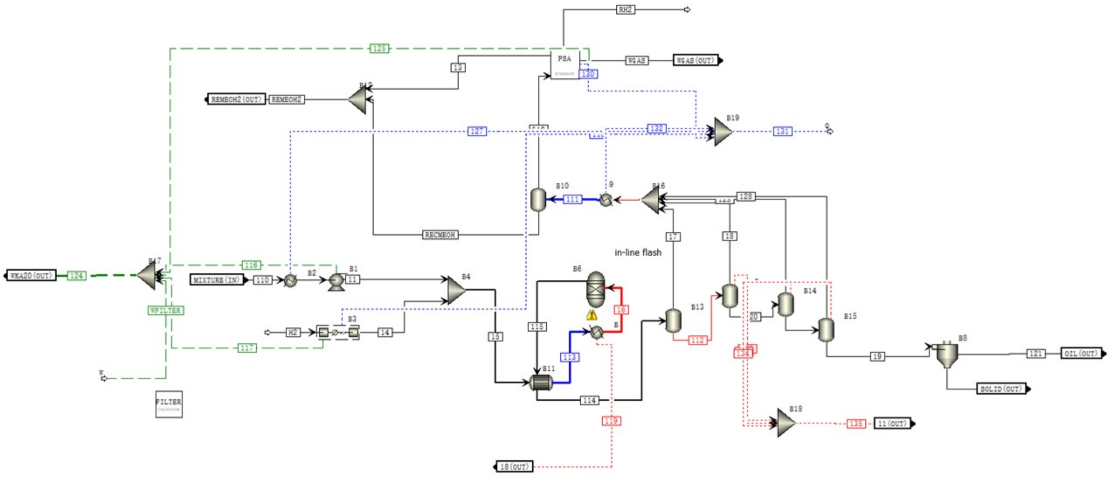


Fig. S2 Aspen Plus simulation flowchart for Catalytic hydrogenolysis (A200) section

Area 300 (A300): Oligomers extraction. Oligomers in the liquid stream from hydrogenolysis are obtained via the liquid-liquid extraction. The process is carried out using n-Hexane in an extraction column, 80 °C, with an n-hexane/lignin oil mass ratio of 3:1. The extraction efficiency is 60% (based on experimental data). After the extraction, n-hexane is separated and recovered using a plate distillation column. The monomer-rich fraction is then sent to Area 400 (A400) for dealkylation.

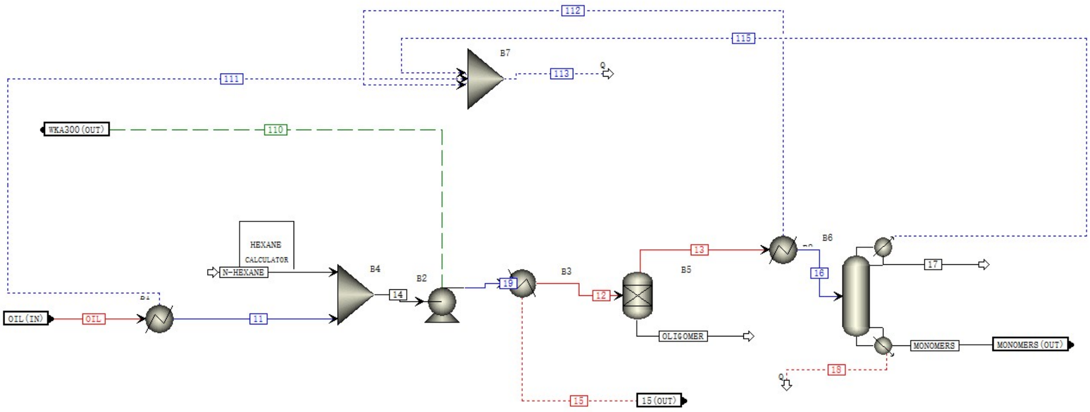


Fig. S3 Aspen Plus simulation flowchart for Oligomers extraction (A300) section

Area 400 (A400): Dealkylation. In this process, propylcatechol is converted to catechol via a gas-phase reaction conducted in a fixed-bed reactor under the atmospheric pressure at 400°C using ZSM-5-40 as the catalyst (weight hour space velocity (WHSV) = 4.2 h^{-1}).[4] Catechol monomers from A300 are mixed with medium pressure steam (266 °C) from A600 before being fed to the dealkylation reactor which is further heated to 400°C using boiler flue gas from A600.

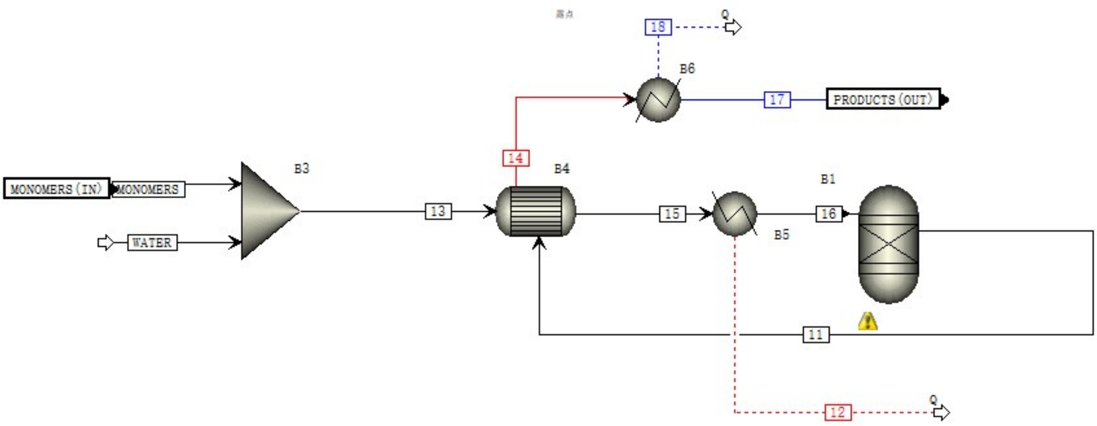


Fig. S4 Aspen Plus simulation flowchart for Dealkylation (A400) section

Area 500 (A500): Separation. The products from A400 are separated to the main product catechol, co-products propanolcatechol and propylene. Firstly the stream is sent to a condenser for quenching, separating product vapors from non-condensable gases (CO_2 and propylene). The stream is then preheated and sent to flash evaporation to remove water, first plate distillation column to remove the remaining water, the resulted propanolcatechol and catechol were further separated by the second plate distillation column to yield products at high purity (99.9%).

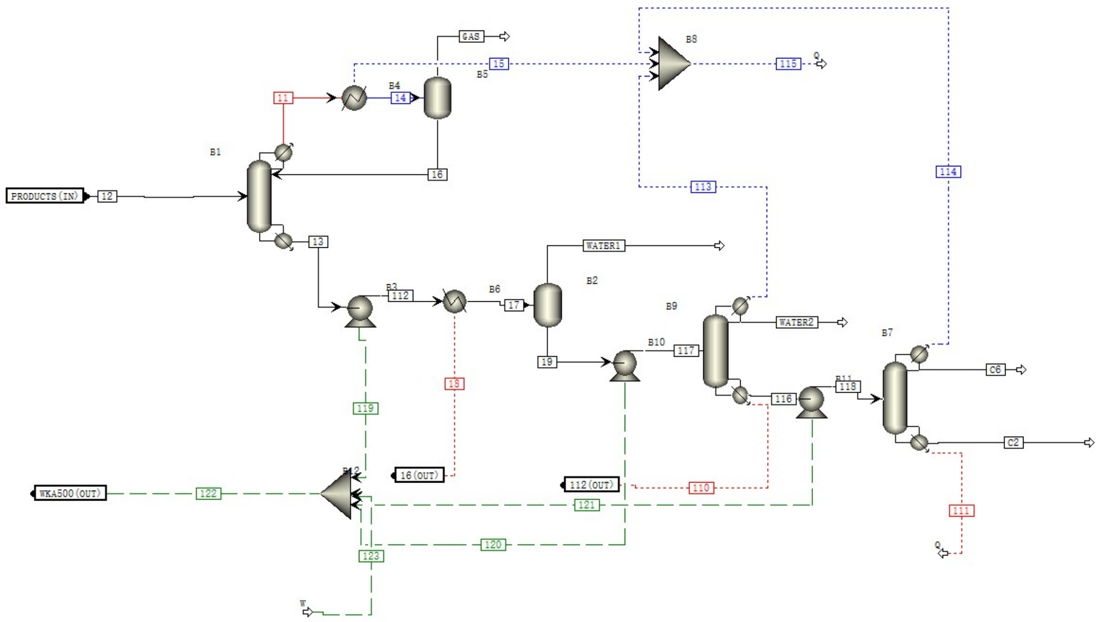


Fig. S5 Aspen Plus simulation flowchart for Separation (A500) section

Area 600 (A600): Combined Heat and Power. The CHP system design follows the U.S. NREL report which primarily consists of a burner, boiler, and turbine system. CHP system normally runs in two modes, either in the heat mode (following heat demand) or in the power mode (following power demand).[5] In this study, heat mode was chosen because the heat demand was significantly higher, which is about 10 times that of electricity. Combustible wastes generated throughout the process including unreacted lignin and waste gases from the A200 are incinerated here to produce steam for thermal energy and electricity required by the plant, such as A100, A200, A300, A400 and A500. This unit primarily consists of a burner, boiler, and turbine system. The combustion is performed with 20% excess air to ensure the complete combustion. Boiler feedwater is sent into the heat exchanger to generate the superheated steam at 454°C and under 60 bar, with the overall efficiency around 80% (steam heat over combustible waste on energy basis). The superheated steam is fed into the turbine system for electricity generation and also is extracted for the use in A400 (13 bar), A100 and A500 (9.5 bar).

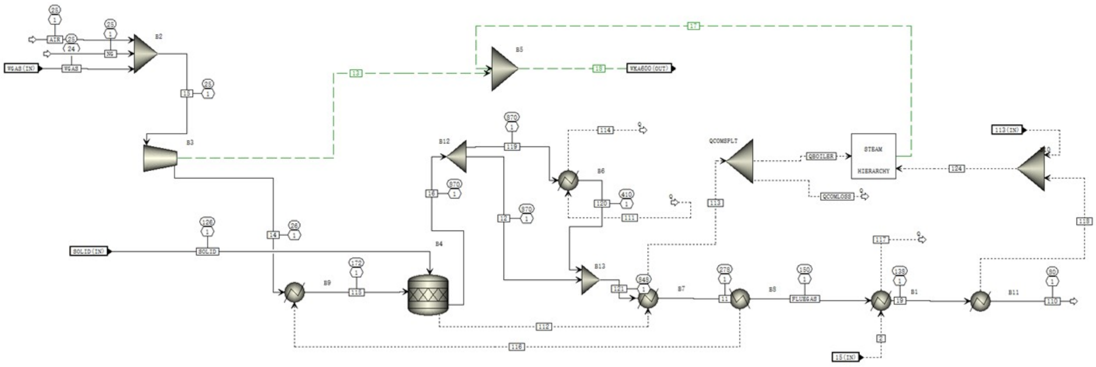


Fig. S6 Aspen Plus simulation flowchart for Cogeneration heat and power (A600) section

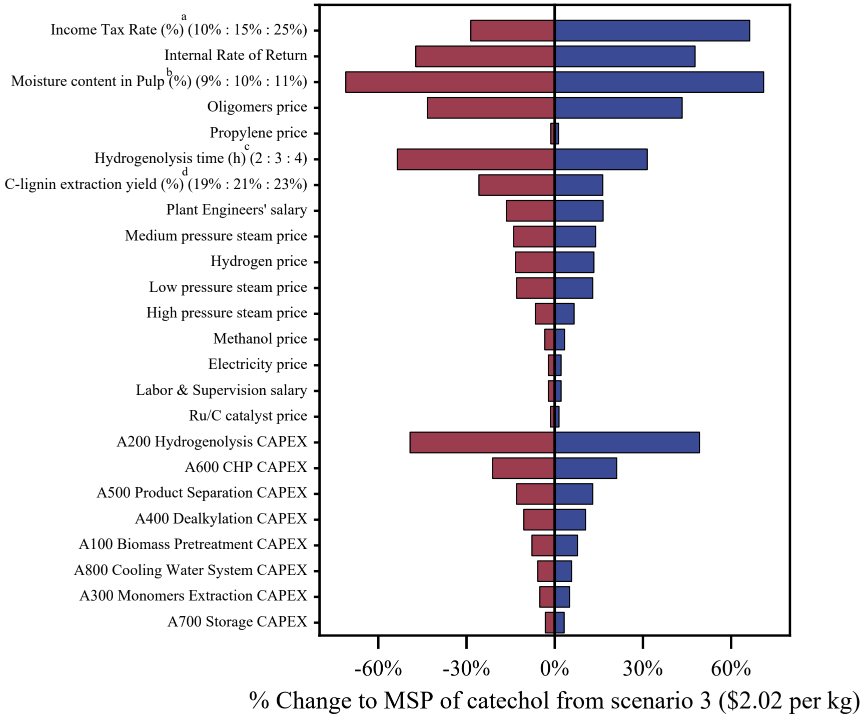
Area 700 (A700): Storage. This area is designated for the bulk storage of chemical materials and products in this process, including methanol, hydrogen, n-hexane, catechol (C6), propanolcatechol (C2), oligomers and propylene.

Area 800 (A800): Cooling Water System. This area provides cooling utilities including cooling water and chilled water for A100 to A600.

Table S2 Operating assumptions and mass balance for principal reaction areas

Process area	condition	Input streams	kg/h	Output streams	kg/h
A100 Pretreatment	70℃, 1.3-1.5 bar, S/L=1:4.4	Castor seed coat (dry)	1500	C-lignin intermediates	406
				pulp	1094
A200 Catalytic hydrogenolysis	200℃, 9~10 MPa, S/L=1:4.4	C-lignin intermediates	406	C-lignin oil	127
				Waste solids	266
				Waste gas	13
A300 Oligomers extraction	80℃, 1 atm, n-hexane/C-lignin oil=3:1	C-lignin oil	127	Oligomers	89
				catechols	38
A400 dealkylation	400 ℃, 1 atm	catechols	38	Catechol (C6)	16
				Propylene	4
				Propanolcatechol (C2)	9
				CO_2	9

Fig. S7 Sensitivity analysis of scenario 3



The local sensitivity analysis was carried out with one-at-a-time (OAT) approach. All variables are varied by 10% unless otherwise stated.

[a] 10%, 15% represent the tax rate of non-resident enterprises and hi-tech sectors mainly under the state support. 25% is the basic enterprise income tax rate in the current tax system.[6]

[b] This range reflects the range of moisture content of pulp.

[c, d] These ranges are based on our experimental experience.

Fig. S8 Carbon efficiency of this process

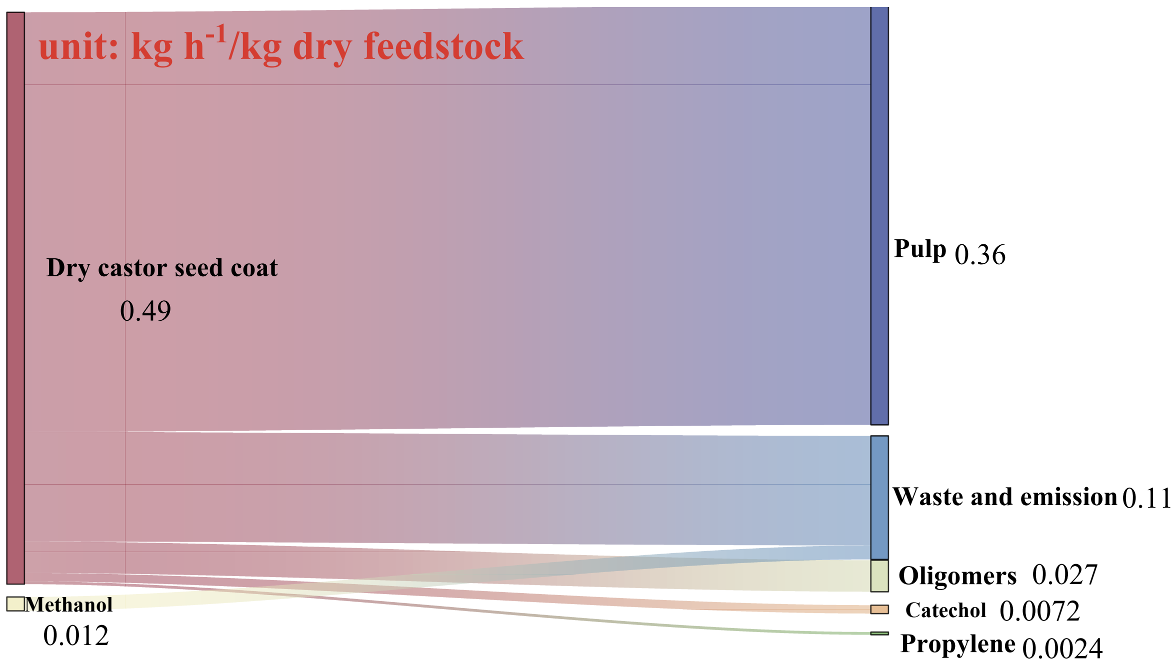


Table S3 full LCA results of fossil-based scenario

Impact category	Unit	Total
Global warming	kg CO_2 eq.	5.72E+00

Stratospheric ozone depletion	kg CFC11 eq.	1.47E-06
Ionizing radiation	kBq Co-60 eq.	2.07E-01
Ozone formation, Human health	kg NOx eq.	1.21E-02
Fine particulate matter formation	kg PM2.5 eq.	8.81E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	1.33E-02
Terrestrial acidification	kg SO_2 eq.	1.72E-02
Freshwater eutrophication	kg P eq.	1.87E-03
Marine eutrophication	kg N eq.	1.72E-04
Terrestrial ecotoxicity	kg 1,4-DCB	1.31E+01
Freshwater ecotoxicity	kg 1,4-DCB	1.73E-01
Marine ecotoxicity	kg 1,4-DCB	2.38E-01
Human carcinogenic toxicity	kg 1,4-DCB	3.84E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	4.56E+00
Land use	m^2a crop eq.	6.82E-02
Mineral resource scarcity	kg Cu eq.	1.09E-02
Fossil resource scarcity	kg oil eq.	2.76E+00
Water consumption	m^3	1.51E-01

Table S4 full LCA results of baseline scenario (S0)

Impact category	Unit	Total
Global warming	kg CO_2 eq.	5.90E+00

Stratospheric ozone depletion	kg CFC11 eq.	9.26E-06
Ionizing radiation	kBq Co-60 eq.	5.51E-02
Ozone formation, Human health	kg NOx eq.	1.26E-02
Fine particulate matter formation	kg PM2.5 eq.	6.12E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	1.28E-02
Terrestrial acidification	kg SO_2 eq.	1.64E-02
Freshwater eutrophication	kg P eq.	1.18E-03
Marine eutrophication	kg N eq.	3.41E-03
Terrestrial ecotoxicity	kg 1,4-DCB	2.60E+00
Freshwater ecotoxicity	kg 1,4-DCB	7.69E-02
Marine ecotoxicity	kg 1,4-DCB	1.05E-01
Human carcinogenic toxicity	kg 1,4-DCB	1.05E-01
Human non-carcinogenic toxicity	kg 1,4-DCB	5.17E+00
Land use	m^2a crop eq.	3.99E-02
Mineral resource scarcity	kg Cu eq.	9.82E-03
Fossil resource scarcity	kg oil eq.	2.20E+00
Water consumption	m^3	1.47E-01

Table S5 full LCA results of scenario 1 (S1)

Impact category	Unit	Total
Global warming	kg CO_2 eq.	2.83E+00

Stratospheric ozone depletion	kg CFC11 eq.	1.17E-06
Ionizing radiation	kBq Co-60 eq.	9.56E-03
Ozone formation, Human health	kg NOx eq.	4.65E-03
Fine particulate matter formation	kg PM2.5 eq.	1.66E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	4.89E-03
Terrestrial acidification	kg SO_2 eq.	4.92E-03
Freshwater eutrophication	kg P eq.	1.91E-04
Marine eutrophication	kg N eq.	1.07E-05
Terrestrial ecotoxicity	kg 1,4-DCB	5.15E-01
Freshwater ecotoxicity	kg 1,4-DCB	2.78E-02
Marine ecotoxicity	kg 1,4-DCB	3.97E-02
Human carcinogenic toxicity	kg 1,4-DCB	2.12E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	9.07E-01
Land use	m^2a crop eq.	3.60E-03
Mineral resource scarcity	kg Cu eq.	8.30E-03
Fossil resource scarcity	kg oil eq.	1.83E+00
Water consumption	m^3	1.47E-01

Table S6 full LCA results of scenario 2 (S2)

Impact category	Unit	Total

Global warming	kg CO_2 eq.	3.18E+00
Stratospheric ozone depletion	kg CFC11 eq.	1.26E-06
Ionizing radiation	kBq Co-60 eq.	1.06E-02
Ozone formation, Human health	kg NOx eq.	5.23E-03
Fine particulate matter formation	kg PM2.5 eq.	1.87E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	5.48E-03
Terrestrial acidification	kg SO_2 eq.	5.41E-03
Freshwater eutrophication	kg P eq.	1.97E-04
Marine eutrophication	kg N eq.	1.19E-05
Terrestrial ecotoxicity	kg 1,4-DCB	5.28E-01
Freshwater ecotoxicity	kg 1,4-DCB	2.81E-02
Marine ecotoxicity	kg 1,4-DCB	4.03E-02
Human carcinogenic toxicity	kg 1,4-DCB	2.26E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	9.04E-01
Land use	m^2a crop eq.	4.16E-03
Mineral resource scarcity	kg Cu eq.	8.37E-03
Fossil resource scarcity	kg oil eq.	2.00E+00
Water consumption	m^3	1.44E-01

Table S7 full LCA results of scenario 3 (S3)

Impact category	Unit	Total

Global warming	kg CO_2 eq.	1.58E+00
Stratospheric ozone depletion	kg CFC11 eq.	1.33E-06
Ionizing radiation	kBq Co-60 eq.	2.32E-02
Ozone formation, Human health	kg NOx eq.	6.11E-03
Fine particulate matter formation	kg PM2.5 eq.	2.73E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	6.28E-03
Terrestrial acidification	kg SO_2 eq.	7.20E-03
Freshwater eutrophication	kg P eq.	3.77E-04
Marine eutrophication	kg N eq.	2.01E-05
Terrestrial ecotoxicity	kg 1,4-DCB	1.15E+00
Freshwater ecotoxicity	kg 1,4-DCB	3.95E-02
Marine ecotoxicity	kg 1,4-DCB	5.47E-02
Human carcinogenic toxicity	kg 1,4-DCB	4.77E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.11E+00
Land use	m^2a crop eq.	1.65E-02
Mineral resource scarcity	kg Cu eq.	8.37E-03
Fossil resource scarcity	kg oil eq.	1.24E+00
Water consumption	m^3	1.46E-01

Table S8 full LCA results of scenario 4 (S4)

Impact category	Unit	Total

Global warming	kg CO_2 eq.	1.05E+00
Stratospheric ozone depletion	kg CFC11 eq.	1.92E-06
Ionizing radiation	kBq Co-60 eq.	2.20E-02
Ozone formation, Human health	kg NOx eq.	6.07E-03
Fine particulate matter formation	kg PM2.5 eq.	2.51E-03
Ozone formation, Terrestrial ecosystems	kg NOx eq.	6.22E-03
Terrestrial acidification	kg SO_2 eq.	6.56E-03
Freshwater eutrophication	kg P eq.	3.61E-04
Marine eutrophication	kg N eq.	1.93E-05
Terrestrial ecotoxicity	kg 1,4-DCB	9.43E-01
Freshwater ecotoxicity	kg 1,4-DCB	3.74E-02
Marine ecotoxicity	kg 1,4-DCB	5.21E-02
Human carcinogenic toxicity	kg 1,4-DCB	4.41E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.04E+00
Land use	m^2a crop eq.	1.53E-02
Mineral resource scarcity	kg Cu eq.	7.93E-03
Fossil resource scarcity	kg oil eq.	9.57E-01
Water consumption	m^3	1.45E-01

Table S9 full LCA results of scenario 5 (S5)

Impact category	Unit	Total

Global warming	kg CO_2 eq.	1.94E-01
Stratospheric ozone depletion	kg CFC11 eq.	7.90E-06
Ionizing radiation	kBq Co-60 eq.	2.61E-02
Ozone formation, Human health	kg NOx eq.	4.64E-03
Fine particulate matter formation	kg PM2.5 eq.	1.45E-02
Ozone formation, Terrestrial ecosystems	kg NOx eq.	4.71E-03
Terrestrial acidification	kg SO_2 eq.	1.04E-01
Freshwater eutrophication	kg P eq.	4.27E-04
Marine eutrophication	kg N eq.	2.19E-05
Terrestrial ecotoxicity	kg 1,4-DCB	1.16E+00
Freshwater ecotoxicity	kg 1,4-DCB	4.04E-02
Marine ecotoxicity	kg 1,4-DCB	5.57E-02
Human carcinogenic toxicity	kg 1,4-DCB	4.66E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.12E+00
Land use	m^2a crop eq.	2.86E-02
Mineral resource scarcity	kg Cu eq.	8.14E-03
Fossil resource scarcity	kg oil eq.	4.46E-01
Water consumption	m^3	1.45E-01

Table S10 full LCA results of scenario 6 (S6)

Impact category	Unit	Total

Global warming	kg CO_2 eq.	1.92E-01
Stratospheric ozone depletion	kg CFC11 eq.	7.90E-06
Ionizing radiation	kBq Co-60 eq.	3.10E-02
Ozone formation, Human health	kg NOx eq.	4.78E-03
Fine particulate matter formation	kg PM2.5 eq.	1.46E-02
Ozone formation, Terrestrial ecosystems	kg NOx eq.	4.86E-03
Terrestrial acidification	kg SO_2 eq.	1.04E-01
Freshwater eutrophication	kg P eq.	4.54E-04
Marine eutrophication	kg N eq.	2.73E-05
Terrestrial ecotoxicity	kg 1,4-DCB	1.31E+00
Freshwater ecotoxicity	kg 1,4-DCB	4.23E-02
Marine ecotoxicity	kg 1,4-DCB	5.84E-02
Human carcinogenic toxicity	kg 1,4-DCB	4.97E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.25E+00
Land use	m^2a crop eq.	2.90E-01
Mineral resource scarcity	kg Cu eq.	8.28E-03
Fossil resource scarcity	kg oil eq.	3.86E-01
Water consumption	m^3	1.46E-01

Table S11 full LCA results of scenario 7 (S7)

Impact category	Unit	Total
Global warming	kg CO_2 eq.	-7.03E-01
Stratospheric ozone depletion	kg CFC11 eq.	7.99E-06
Ionizing radiation	kBq Co-60 eq.	1.75E-02
Ozone formation, Human health	kg NOx eq.	2.27E-03
Fine particulate matter formation	kg PM2.5 eq.	1.32E-02
Ozone formation, Terrestrial ecosystems	kg NOx eq.	2.35E-03
Terrestrial acidification	kg SO_2 eq.	1.01E-01
Freshwater eutrophication	kg P eq.	2.92E-04
Marine eutrophication	kg N eq.	2.67E-05
Terrestrial ecotoxicity	kg 1,4-DCB	9.10E-01
Freshwater ecotoxicity	kg 1,4-DCB	3.33E-02
Marine ecotoxicity	kg 1,4-DCB	4.60E-02
Human carcinogenic toxicity	kg 1,4-DCB	2.75E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.08E+00
Land use	m^2a crop eq.	2.84E-01
Mineral resource scarcity	kg Cu eq.	8.41E-03
Fossil resource scarcity	kg oil eq.	2.16E-01
Water consumption	m^3	1.44E-01

Table S12 full LCA results of scenario 8 (S8)

Impact category	Unit	Total
Global warming	kg CO_2 eq.	-1.32E+00
Stratospheric ozone depletion	kg CFC11 eq.	7.81E-06
Ionizing radiation	kBq Co-60 eq.	-2.66E-02
Ozone formation, Human health	kg NOx eq.	1.15E-03
Fine particulate matter formation	kg PM2.5 eq.	1.21E-02
Ozone formation, Terrestrial ecosystems	kg NOx eq.	1.22E-03
Terrestrial acidification	kg SO_2 eq.	9.93E-02
Freshwater eutrophication	kg P eq.	2.02E-04
Marine eutrophication	kg N eq.	2.11E-05
Terrestrial ecotoxicity	kg 1,4-DCB	4.48E+00
Freshwater ecotoxicity	kg 1,4-DCB	2.41E-01
Marine ecotoxicity	kg 1,4-DCB	3.00E-01
Human carcinogenic toxicity	kg 1,4-DCB	3.67E-02
Human non-carcinogenic toxicity	kg 1,4-DCB	2.00E+00
Land use	m^2a crop eq.	2.83E-01
Mineral resource scarcity	kg Cu eq.	1.26E-02
Fossil resource scarcity	kg oil eq.	-7.83E-03
Water consumption	m^3	1.30E-01

Table S13 Emission factors of natural gas combustion for stationary applications (grams per mmBtu of fuel burned).[7]

	small industrial boiler	small turbine
VOC	2.54E+00	1.06E+00
CO	2.50E+01	4.13E+01
NOx	4.11E+01	3.20E+01
PM10	3.51E+00	3.58E+00
PM2.5	3.51E+00	3.58E+00
SOx	2.69E-01	2.69E-01
BC	5.79E-01	1.04E-01
OC	1.50E+00	2.43E+00
CH_4	1.06E+00	1.06E+00
N_2O	3.50E-01	1.02E-01
CO_2	5.94E+04	5.93E+04

Table S14 Life cycle inventory for production of 1 kg 5% Ru/C catalyst. [8]

Inputs from nature	**Total amount**	**Allocated amount**	**Unit**

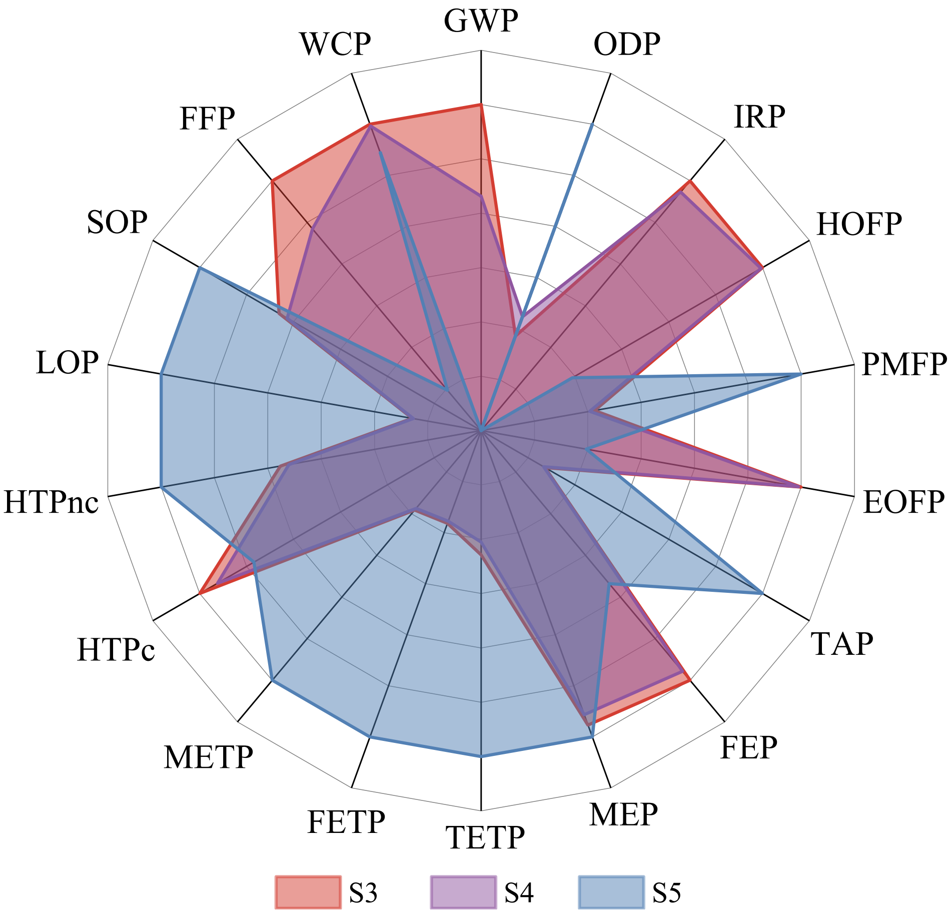
Water, process, unspecified natural origin/m³	5.85E-03	5.85E-03	kg
Materials/fuels	**Total amount**	**Allocated amount**	**Unit**
Activated carbon, granular {GLO}| market for activated carbon, granular | Cut-off, U	9.42E-01	9.42E-01	kg
Water, deionised, from tap water, at user [3]| market for water, deionised, from tap water, at user | Cut-off, U	9.45E-01	9.45E-01	kg
Nitrogen, liquid {RER}| market for | Cut-off, U	2.59E-03	2.59E-03	kg
Ru	2.85E-02	2.85E-02	kg
Chlorine, gaseous {RER}| market for | Cut-off, U	2.97E-02	2.97E-02	kg
Electricity/heat	**Total amount**	**Allocated amount**	**Unit**
Heat, district or industrial, natural gas {RoW}| heat production, natural gas, at industrial furnace >100kW | Cut-off, U	3.12E+02	3.12E+02	MJ
Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | Cut-off, U	2.52E+00	2.52E+00	MJ
Electricity, medium voltage {CN}| market group for | Cut-off, U	8.73E+01	8.73E+01	kJ

Table S15 Life cycle inventory for production of 1 kg green hydrogen.[9]

Avoided products	**Total amount**	**Allocated amount**	**Unit**

Oxygen, liquid {RoW}| market for | Cut-off, U	8	8	kg
Inputs from nature	**Total amount**	**Allocated amount**	**Unit**
Water, salt, ocean	9	9	kg
Materials/fuels	**Total amount**	**Allocated amount**	**Unit**
Activated carbon, granular {GLO}| market for activated carbon, granular | Cut-off, U	9.94E-6		kg
Reinforcing steel {GLO}| market for | Cut-off, U	1.11E-04		kg
Polyvinylfluoride, film {GLO}| market for | Cut-off, U	1.76E-5		kg
Copper {GLO}| market for | Cut-off, U	4.97E-6		kg
Platinum {GLO}| market for | Cut-off, U	8.0E-8		kg
Titanium, primary {GLO}| market for | Cut-off, U	5.83E-04		kg
Aluminium, primary, ingot {RoW}| market for | Cut-off, U	2.98E-5		kg
Electricity/heat	**Total amount**	**Allocated amount**	**Unit**
Electricity, high voltage {CN-HB}| electricity production, wind, >3MW turbine, onshore | Cut-off, U	49.02	49.02	kWh

Fig S9 Full LCA analysis results of S3-S5



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