Supplementary Material for: Integrated technoeconomic and environmental assessment of biogenic polyurethane production

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S.1. Economic evaluation data and results

Table S.1. List of equipment and cost estimation for the economic assessment

Tanks

Name	Type	Design variable: Volume (m3)	Cost ($)	Updated cost ($2024)	Number of units
Tank 1	Jacketed Vertical stirred tank	18.5	45,573	62,897	1
Tank 2	Jacketed Vertical stirred tank	19.0	46,370	63,997	1
Ferm1	Foundation-mounted tank with stirring and temperature control	200.0	1,306,537	1,803,207	4
Crystal	Vertical stirred tank with temperature control	21.4	2,400,710	3,313,321	6
React1	Jacketed Vertical stirred tank	1.0	6,840	9,440	1
Tank4	Vertical stirred tank with temperature control	15.0	39,765	54,882	1
Tank5	Vertical stirred tank with temperature control	15.0	39,765	54,882	1
AccTank2	Vertical stirred tank with temperature control	20.5	48,720	67,241	1
React2	Vertical stirred tank with temperature control	18.8	46,092	63,613	1
Tank6	Vertical stirred tank with temperature control	9.9	30,288	41,801	1
React3	Vertical stirred tank with temperature control	10.0	30,602	42,235	1
React4	Jacketed Vertical stirred tank	0.6	4,918	6,787	1
React5	Jacketed Vertical stirred tank	0.1	1,761	2,430	1

Heat exchangers

Name	Type	Design variable: Surface (m2)	Cost ($)	Updated cost ($2024)	Number of units
HX1	Shell and tube	3.99	2,312	3,190	1
HX2	Shell and tube	40.92	67,803	93,578	1
HX3	Double pipe	0.25	37	51	1
HX4	Not needed	0	-	-	-
HX5	Shell and tube	23.79	33,158	45,763	1
HX6	Double pipe	0.10	9	12	1

HX7	Double pipe	0.29	46	63	1
HX8	Double pipe	0.31	52	72	1
HX9	Shell and tube	6.46	4,740	6,542	1
HX10	Double pipe	0.02	1	2	1
HX11	Not needed	0	-	-	-
HX12	Double pipe	0.01	0	1	1
HX13	Shell and tube	60.71	99,347	137,113	1
HX14	Double pipe	0.06	5	7	1
HX15	Double pipe	0.09	8.48	12	1
HX16	Double pipe	0.36	63.95	88	1
HX17	Shell and tube	2.28	1,004.58	1,386	1
HX18	Double pipe	0.45	89.68	124	1
HX19	Double pipe	0.59	135.24	187	1
HX20	Double pipe	0.51	106.84	147	1
HX21	Shell and tube	4.27	2,558.16	3,531	1
HX22	Double pipe	0.39	71.50	99	1
HX23	Shell and tube	1.96	802.00	1,107	1
HX24	Double pipe	0.30	49.77	69	1
HX25	Double pipe	0.22	31.20	43	1
HX26	Shell and tube	15.59	17,657.48	24,370	1
HX27	Shell and tube	11.61	11,367.55	15,689	1
HX28	Double pipe	0.03	1.62	2	1
HX29	Not needed	0.00	-	-	-
HX30	Not needed	0	-	-	-
HX31	Shell and tube	0.59	134.30	185	1
HX32	Shell and tube	1.28	423.24	584	1
HX33	Double pipe	0.16	18.65	26	1
HX34	Double pipe	0.12	12.38	17	1
HX35	Double pipe	0.44	85.58	118	1
HX36	Double pipe	0.19	24.43	34	1
HX37	Double pipe	0.17	21.76	30	1
Evapor1	Evaporator	43.02	71,146.20	98,192	1
Cond_DC1	Shell and tube	15.35	17,249.82	23,807	1
Evap_DC1	Evaporator	1.40	483.24	667	1
Cond_DC2	Conde	1.70	648.18	895	1
Evap_DC2	Evaporator	0.12	12.93	18	1
Cond_DC3	Shell and tube	7.75	6,220.40	8,585	1
Evap_DC3	Evaporator	3.54	1,936.33	2,672	1
Cond_TFD	Shell and tube	0.32	52.79	73	1

Pressure changers (liquid)					
Name	**Type**	**Design variable: Flow (gal min^{-1})**	**Cost ($)**	**Updated cost ($2024)**	**Number of units**
Pump 1	Piston medium	73.4	31,900	44,027	1
Pump2	Progressive Cavity, Small	1.0	4,239	5,850	1

Pump3	Progressive Cavity, Medium	2.4	4,643	6,408	1
Pump4	Progressive Cavity, Medium	3.8	5,420	7,481	1
Pump5	Progressive Cavity, Medium	4.5	5,765	7,956	1
Pump6	Progressive Cavity, Small	0.8	4,207	5,807	1
Vacpump	Vacuum pump blower dry seal, medium	74.8	12,299	16,974	1
Pump7	Progressive Cavity, Small	0.3	4,062	5,606	1
Pump 1	Piston medium	73.4	31,900	44,027	1
Pump2	Progressive Cavity, Small	1.0	4,239	5,850	1

Pressure changers (gas)						
Name	**Type**	**Pressure range (bar)**	**Design variable: Power input (gal min-1)**	**Cost ($)**	**Updated cost ($2024)**	**Number of units**
Blower 1	Compressor	< 8 bar	92.66	31,900	44,027	1
Blower 2	Compressor	< 8 bar	1.35	4,239	5,850	1
Comp1	Compressor	< 8 bar	3.47	4,643	6,408	1
Comp2	Compressor	< 8 bar	3.42	5,420	7,481	1
Comp3	Compressor	< 8 bar	0.21	5,765	7,956	1
Blower3	Compressor	< 8 bar	0.14	4,207	5,807	1
Comp4	Compressor	> 8 bar	462.51	12,299	16,974	1
Exp1	Turbine	< 8 bar	115.59	4,062	5,606	1
Ref Ammonia	Compressor	< 8 bar	36.50	31,900	44,027	1
Ref Nitrogen 1	Compressor	< 8 bar	2105.75			
Ref Nitrogen 2	Compressor	< 8 bar	888.57	4,239	5,850	1

Columns						
Name	**Type**	**Weight (kg)**	**Internals ($)**	**Cost ($)**	**Updated cost ($2024)**	**Number of units**
Abs_C1	Vertical vessel	1109	7637	37,035	51,113	1
Dis_C1	Vertical vessel	568	4481	20,837	28,759	1
Dis_C2	Vertical vessel	1855	9219	55,426	76,496	1
Dis_C3	Vertical vessel	553	4451	20,419	28,181	1
Abs_C2	Vertical vessel	538	4422	20,017	27,627	1
DisTF	Vertical vessel	151	1850	6,970	9,619	
Flash1	Vertical vessel	166	1873	7,410	10,227	1

Other instrumentation			
Name	**Type**	**Updated cost ($2024)**	**Number of units**
Oven	Curing oven	12,000	4
Crystal drier	Vessel	Cost as part of auxiliary material	1
Solid separators	Filters and centrifugation	Cost as part of auxiliary material	10

Table S.2. List of delivered duty free prices for raw materials and utilities used for the economic assessment

Operation time basis	*7008 h year $^{-1}$*			
	Price		Annual cost ($/year)	Reference
Raw Materials				
Water (filtered)	5.70	$ m^{-3}	1,407,179	[1]
Sugarcane molasses	193.90	$ ton^{-1}	5,698,362	[2]
Activated carbon	2.55	$ ton^{-1}	701	[3]
Sulfuric acid	130.00	$ ton^{-1}	297,957	[4]
Peptone	6000.00	$ ton^{-1}	417,692	[5]
Sodium chloride	120.00	$ ton^{-1}	8,354	[6]
Yeast extract	900.00	$ ton^{-1}	31,327	[7]
Sodium hydroxide	240.00	$ ton^{-1}	789,227	[8]
Threonine	2021.00	$ ton^{-1}	90,442	[9]
Nitrogen	0.05	$ m^{-3}	139,991	[10]
Ammonium hydroxide	280.00	$ ton^{-1}	372,151	[11]
Hydrogen chloride	120.00	$ ton^{-1}	52,051	[12]
Carbon monoxide	10.00	$ m^{-3}	5,804,776	[13]
Chlorine	400.00	$ ton^{-1}	667,425	[14]
Pyridoxal phosphate	50000.00	$ ton^{-1}	10,862	[15]
Monopotassium phosphate	1750.00	$ ton^{-1}	121,528	[16]
E-coli bacteria	310.00	$ vial^{-1}	1,043	[17]
Butanol	1250.00	$ ton^{-1}	2,470,338	[18]
Ethanol	1050.00	$ ton^{-1}	2,458,316	[19]
Ortho dichlorobenzene	1910.00	$ ton^{-1}	1,552,157	[20]
Castor oil	1585.00	$ ton^{-1}	3,534,097	[21]
Triethylenediamine	9000.00	$ ton^{-1}	602,022	[22]
Utilities				
Natural gas	34.70	$ MWh^{-1}	5,109,597.32	[23]
Water (refrigeration)	0.05	$ m^{-3}	59,885.56	[24]
Electricity (EU average)	0.18	$ kWh^{-1}	5,019,713.3	[25]

Table S.3. Total capital cost estimation for the PU resin production process

Total cost of equipment (C_E)	$C_E = 8.8\ M\$$
Inside Battery Limits Investment (C_{ISBL})	$C_{ISBL} = C_E\left[(1+f_p)f_m + (f_{er}+f_{el}+f_i+f_c+f_s+f_l)\right]$
Piping (f_p)	0.8
Material (f_m)	1
Equipment erection (f_{er})	0.3
Electrical work (f_{el})	0.2
Instrumentation (f_i)	0.3
Civil engineering (f_c)	0.3
Structures and buildings (f_s)	0.2
Lagging (f_l)	0.1
	$C_{ISBL} = 28.1\ M\$$
Total Fixed Capital Cost ($CAPEX$)	$CAPEX = C_{ISBL}(1+f_{OS})(1+f_{D\&E}+f_X)$
Offsites cost (f_{OS})	0.3
Design and Engineering ($f_{D\&E}$)	0.3
Contingency (f_X)	0.1
	$CAPEX = 51.1\ M\$$
Annualized capital cost (ACC)	$ACC = ACCR \times CAPEX$
Annual capital change ratio ($ACCR$)	$ACCR = \dfrac{i(1+i)^n}{(1+i)^n - 1}$
Interest rate (i)	0.085
Plant lifetime (n)	$25\ years$
	$ACC = 5.0\ M\$$
Working Capital (WC)	$WC = 0.15 \times CAPEX = 7.7 M\$$

Table S.4. Operating cost estimation for the PU resin production process

Total Operating Cost (OPEX)	$OPEX = C_{VCP} + C_{FCP}$
Variable cost of production (C_{VCP})	$C_{VCP} = C_{RM} + C_U$
Cost of raw materials (C_{RM})	26.5 $M\$ \, yr^{-1}$
Cost of Utilities (C_U)	10.1 $M\$ \, yr^{-1}$
	$C_{VCP} = 36.7 \, M\$ \, yr^{-1}$
Fixed cost of production (C_{FCP})	$C_{FCP} = C_l + C_S + C_{SO} + C_M + C_{LR} + C_{R\&D} + C_{EC}$
Operating labor (C_l)	$C_l = N_{WS} \times N_s \times S = 1.9 \, M\$ \, yr^{-1}$
Number Workstations (N_{WS})	8
Number of shifts (N_s)	5
Average salary (S)	48,948 $\$ \, yr^{-1}$
Supervision (C_S)	$C_S = 0.25 \times C_l$
Direct salary overhead (C_{SO})	$C_{SO} = 0.5 \times (C_l + C_S)$
Maintenance (C_M)	$C_M = 0.03 \times C_{ISBL}$
Land rent (C_{LR})	$C_{LR} = 0.015 \times (C_{ISBL} \times (1 + f_{OS})$
Research and development ($C_{R\&D}$)	$C_{R\&D} = 0.65 \times (C_l + C_S + C_M)$
Environmental charges (C_{EC})	$C_{EC} = 0.01 \times (C_{ISBL} \times (1 + f_{OS})$
	$C_{FCP} = 8.2 \, M\$ \, yr^{-1}$
Marketing (C_{Mark})	$C_{Mark} = 0.03 \times OPEX$
	$OPEX = 44.9 \, M\$ \, yr^{-1}$
Total annualized cost (TAC)	$TAC = ACC + OPEX = 49.9 \, M\$ \, yr^{-1}$

Table S.5. Economic performance of the PU manufacturing process variation with product selling price.

Selling price ($ ton^{-1})	Multiplier fossil-PU price	Sales revenue (M$ yr^{-1})	Gross profit (M$ yr^{-1})	Taxes (M$ yr^{-1})	Net profit (M$ yr^{-1})	Return of investment (yr^{-1})	Payout time (yr)	
3000	1	11.7	-33.2	0.0	0.0	-	-	
3,750	1.25	14.6	-30.3	0.0	0.0	-	-	
4,500	1.5	17.5	-27.4	0.0	0.0	-	-	
5,250	1.75	20.4	-24.5	0.0	0.0	-	-	
6,000	2	23.3	-21.6	0.0	0.0	-	-	
6,750	2.25	26.2	-18.7	0.0	0.0	-	-	
7,500	2.5	29.2	-15.7	0.0	0.0	-	-	
8,250	2.75	32.1	-12.8	0.0	0.0	-	-	
9,000	3	35.0	-9.9	0.0	0.0	-	-	
9,750	3.25	37.9	-7.0	0.0	0.0	-	-	
10,500	3.5	40.8	-4.1	0.0	0.0	-	-	
11,250	3.75	43.7	-1.2	0.0	0.0	-	-	
11,547	**3.85**	**44.9**	**0.0**	**0.0**	**0.0**	**-**	**-**	***BP****
12,000	4	46.7	1.8	0.2	1.6	0.03	37.3	
12,750	4.25	49.6	4.7	0.9	3.8	0.06	15.6	
13,500	4.5	52.5	7.6	1.6	6.0	0.10	9.9	
14,250	4.75	55.4	10.5	2.4	8.1	0.14	7.2	
15,000	5	58.3	13.4	3.1	10.3	0.18	5.7	
15,750	5.25	61.2	16.3	3.8	12.5	0.21	4.7	
16,500	5.5	64.2	19.3	4.6	14.7	0.25	4.0	
17,250	5.75	67.1	22.2	5.3	16.9	0.29	3.5	
18,000	6	70.0	25.1	6.0	19.1	0.32	3.1	

*Breakeven point

Table S.6. Net present value (NPV) calculations for the economic activity assuming a selling price for the bio-PU five times the average selling price of fossil-PU, and a discount rate of 10%.

Selling price for the bio-PU = 15,000 $/ton (x5 fossil-PU price)

Discount rate = 0.1

Year	Fixed capital (M$)	Working Capital (M$)	Depreciation (linear) (M$ yr^{-1})	Cash Inflow (M$ yr^{-1})	Discount factor	NPV annual (M$)	Cumulated NPV (M$)
0	51.12	7.67	0	0	1	-58.8	-58.8
1	0	0	2.04	13.42	0.909	12.2	-46.6
2	0	0	2.04	13.42	0.826	11.1	-35.5
3	0	0	2.04	13.42	0.751	10.1	-25.4
4	0	0	2.04	13.42	0.683	9.2	-16.2
5	0	0	2.04	13.42	0.621	8.3	-7.9
6	0	0	2.04	13.42	0.564	7.6	-0.3
7	**0**	**0**	**2.04**	**13.42**	**0.513**	**6.9**	**6.6**
8	0	0	2.04	13.42	0.467	6.3	12.8
9	0	0	2.04	13.42	0.424	5.7	18.5
10	0	0	2.04	13.42	0.386	5.2	23.7
11	0	0	2.04	13.42	0.350	4.7	28.4
12	0	0	2.04	13.42	0.319	4.3	32.7
13	0	0	2.04	13.42	0.290	3.9	36.6
14	0	0	2.04	13.42	0.263	3.5	40.1
15	0	0	2.04	13.42	0.239	3.2	43.3
16	0	0	2.04	13.42	0.218	2.9	46.3
17	0	0	2.04	13.42	0.198	2.7	48.9
18	0	0	2.04	13.42	0.180	2.4	51.3
19	0	0	2.04	13.42	0.164	2.2	53.5
20	0	0	2.04	13.42	0.149	2.0	55.5
21	0	0	2.04	13.42	0.135	1.8	57.3
22	0	0	2.04	13.42	0.123	1.6	59.0
23	0	0	2.04	13.42	0.112	1.5	60.5
24	0	0	2.04	13.42	0.102	1.4	61.8
25	0	0	2.04	13.42	0.092	1.2	63.1

S.2. Lifecycle inventory data for polyisocyanate prepolymer and bio-PU resin final product

Table S.7. Lifecycle inventory for the biogenic PDI-T manufacturing process in a cradle-to-gate system boundary. The inventory is referred to the functional unit, i.e., **'1 kg of polyisocyanate produced by the proposed integrated process'**.

Item	Input Value	Units	SimaPro module
Inputs from nature			
Air	139.10	kg	Air
Water (cooling)	0.45	m^3	Water, cooling, unspecified natural origin, Europe without Switzerland
Inputs from Technosphere: materials/fuels			
Water	63.22	kg	Water, completely softened {RoW}| market for water, completely softened | Cut-off, U
Molasses	11.48	kg	Molasses, market mix, at regional storage {BE} Economic, U
Activated carbon	0.11	kg	Activated carbon, granular {GLO}| market for activated carbon, granular | Cut-off, U
Sulfuric acid	0.90	kg	Sulfuric acid {RER}| market for sulfuric acid | Cut-off, U
Peptone	0.04	kg	Protein pea {GLO}| market for protein pea | Cut-off, S
Sodium chloride	0.04	kg	Sodium chloride, powder {GLO}| market for sodium chloride, powder | Cut-off, U
Yeast extract	0.02	kg	Fodder yeast {GLO}| market for fodder yeast | Cut-off, S
Sodium hydroxide	2.05	kg	Sodium hydroxide, without water, in 50% solution state {GLO}| market for sodium hydroxide, without water, in 50% solution state | Cut-off, U
Threonine	0.03	kg	ThreAMINO®, 98.5% L-Threonine, at Evonik plant {HU} Economic, S
Nitrogen	2.20	kg	Nitrogen, liquid {RER}| market for nitrogen, liquid | Cut-off, U
Ammonium hydroxide	0.84	kg	Ammonium sulfate {RER}| market for ammonium sulfate | Cut-off, U
Hydrogen chloride	0.27	kg	Hydrochloric acid, without water, in 30% solution state {RER}| market for hydrochloric acid, without water, in 30% solution state | Cut-off, U
Carbon monoxide	0.42	kg	Carbon monoxide {RER}| market for carbon monoxide | Cut-off, U
Chlorine	1.05	kg	Chlorine, gaseous {RER}| market for chlorine, gaseous | Cut-off, U
Pyridoxal phosphate	1.37 E-4	kg	Enzymes {RER}| enzymes production | Cut-off, U
Monopotassium phosphate	0.04	kg	Potassium carbonate {GLO}| market for potassium carbonate | Cut-off, U
Butanol	1.24	kg	1-butanol {GLO}| market for 1-butanol | Cut-off, U
Ethanol	1.47	kg	Ethanol, without water, in 99.7% solution state, from ethylene {RER}| market for ethanol, without water, in 99.7% solution state, from ethylene | Cut-off, U
Ortho dichlorobenzene	0.51	kg	O-dichlorobenzene {RER}| market for o-dichlorobenzene | Cut-off, U

Infrastructure (chemical plant)	2.55 E-10	p	Chemical factory, organics {RER}| chemical factory construction, organics | Cut-off, U
Inputs from Technosphere: electricity/heat			
Electricity supply	16.47	kWh	Electricity, medium voltage {RER}| market group for electricity, medium voltage | Cut-off, U*
Natural gas supply	5.43	m^3	Natural gas, high pressure {Europe without Switzerland}| market group for natural gas, high pressure | Cut-off, U**
Natural gas burning	4.22	kg	Module created to assign emissions (CO_2, water and air) to the combustion of 1 kg natural gas
Emissions to air			
Oxygen	7.58	kg	Oxygen
Nitrogen	33.37	kg	Nitrogen
Carbon dioxide	3.27	kg	Carbon dioxide
Water	0.01	kg	Water
Hydrochloric acid	0.04	kg	Hydrochloric acid
Argon	4.40 E-1	kg	Argon
Emissions to water			
Water	94.12	kg	Water
Sugars	8.24	kg	Sugars
Ammonia	0.01	kg	Ammonia
Sodium Chloride	1.13	kg	Sodium Chloride
Peptone and yeast	0.05	kg	Corn dust (biomass)
Sodium sulphate	0.05	kg	Sodium sulphate
Lysine	0.50	kg	6-aminohexanoic acid
Carbon dioxide	0.26	kg	Carbon dioxide
Carbon monoxide	9.30 E-4	kg	Carbon monoxide
Chlorine	8.18 E-8	kg	Chlorine
Potassium phosphate	0.03	kg	Tripotassium phosphate
1,5-pentanediamine	0.03	kg	1,3-Propanediamine
Butanol	1.24	kg	1-Butanol
Dichlorobenzene	0.51	kg	4-Bromo-1,2-dichlorobenzene
Isocyanate	0.02	kg	Diisocyanates
Outputs to Technosphere: Waste and emissions to treatment			
Waste water	0.11	m^3	Wastewater, average {Europe without Switzerland}| market for wastewater, average | Cut-off, S
Sodium sulphate	1.45	kg	Sodium sulphate (wfr)/RER
Activated Carbon	0.11	kg	Catalyst, used (wfr)/RER
Solids from molasses	0.57	kg	Filter dust (wfr)/RER
Wet biomass	0.73	kg	Biowaste {RoW}| market for biowaste | Cut-off, U

* In renewable energy assumptions: Electricity, high voltage {CH}| electricity, high voltage, wind power, import from Germany | Cut-off, U

** In renewable energy assumptions: Heat, onsite boiler, hardwood mill average, NE-NC/MJ/RNA

Table S.8. Lifecycle inventory for the bio-PU manufacturing process in a cradle-to-gate system boundary. The inventory is referred to the functional unit, i.e., **'1 kg of polyurethane resin produced by the proposed integrated process'**.

Item	Input Value	Units	SimaPro module
Inputs from nature			
Air	0.03	kg	Air
Water (cooling)	2.00 E-3	m^3	Water, cooling, unspecified natural origin, Europe without Switzerland
Inputs from Technosphere: materials/fuels			
Castor oil	0.57	kg	Palm oil, refined {GLO}| market for palm oil, refined | Cut-off, U. User edited replacing palm tree feedstock for castor bean in a yield of 2.5 kg castor bean per kg castor oil.
Biogenic PDI-T	0.41	kg	User defined PDI-T biological route
Triethylenediamine	0.02	kg	Triethanolamine {GLO}| market for triethanolamine | Cut-off, U
Infrastructure (chemical plant)	5.11 E-11	p	Chemical factory, organics {RER}| chemical factory construction, organics | Cut-off, U
Inputs from Technosphere: electricity/heat			
Electricity supply	16.47	kWh	Electricity, medium voltage {RER}| market group for electricity, medium voltage | Cut-off, U
Natural gas supply	2.00 E-3	m^3	Natural gas, high pressure {Europe without Switzerland}| market group for natural gas, high pressure | Cut-off, U
Natural gas burning	1.55 E-3	kg	Module created to assign emissions (CO_2, water and air) to the combustion of 1 kg natural gas

* In renewable energy assumptions: Electricity, high voltage {CH}| electricity, high voltage, wind power, import from Germany | Cut-off, U

** In renewable energy assumptions: Heat, onsite boiler, hardwood mill average, NE-NC/MJ/RNA

Table S.9. LCA results (kg CO_2-eq) for the Molasses pretreatment (stage A) within the production of 1kg of bio-PDI-T prepolymer.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land transformation	CO_2 uptake

TOTAL	4.48	4.09	0.41	4.15E-03	-2.24E-02
Direct emissions (process)	0.00	0.00	0.00	0.00E+00	0.00E+00
Water SC	0.01	0.01	1.65E-03	3.04E-05	-1.16E-03
Molasses SC	3.03	2.64	0.39	3.66E-03	-9.29E-03
Activated carbon SC	0.37	0.37	3.51E-03	1.99E-04	-3.92E-03
Sulfuric acid SC	0.11	0.11	0.01	1.03E-04	-4.52E-03
Sodium hydroxide SC	0.03	0.03	9.26E-04	4.94E-05	-7.88E-04
Chemical factory	0.01	0.01	6.85E-04	1.19E-05	-8.01E-04
Natural gas SC	0.20	0.20	8.60E-04	6.73E-05	-7.47E-04
Electricity (EU average)	0.01	0.01	1.64E-03	3.00E-05	-1.20E-03
Heating (combustion)	0.71	0.71	0.00	0.00	0.00
Sodium sulphate SC	0.00	0.00	0.00	0.00	0.00
Catalysts SC	0.00	0.00	0.00	0.00	0.00
Waste treatment	0.00	0.00	0.00	0.00	0.00

Table S.10. LCA results (kg CO_2-eq) for the L-lysine HCl synthesis (stage B) within the production of 1kg of bio-PDI-T prepolymer.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land transformation	CO_2 uptake
TOTAL	17.25	17.05	0.41	2.39E-03	-0.21
Direct emissions (process)	3.03	3.03	0.00	0.00	0.00
Water SC	7.90E-04	7.62E-04	0.00	1.64E-06	-6.25E-05
Threonine SC	0.07	0.11	0.09	1.42E-04	-0.14
Ammonium salt SC	1.00	1.00	0.04	7.09E-04	-0.04
HCl SC	0.14	0.14	0.01	2.27E-04	-0.01
Chemical factory	0.01	0.01	0.00	1.19E-05	-8.01E-04
Natural gas SC	2.74	2.74	0.01	9.25E-04	-0.01
Electricity (EU average)	0.15	0.14	0.02	3.60E-04	-0.01
Heating (combustion)	9.85	9.85	0.00	0.00	0.00
Waste treatment	0.26	0.02	0.24	9.03E-06	-7.06E-04

Table S.11. LCA results (kg CO_2-eq) for the Phosgene synthesis (stage D) within the production of 1kg of bio-PDI-T prepolymer.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land	CO_2 uptake

				transformation	
TOTAL	1.46	1.42	0.15	2.94E-03	-0.12
Direct emissions (process)	0.00	0.00	0.00	0.00	0.00
Water SC	1.13E-06	1.13E-06	2.52E-08	2.36E-09	-1.97E-08
Sodium hydroxide SC	9.80E-04	9.73E-04	3.50E-05	1.87E-06	-2.98E-05
Carbon monoxide SC	0.81	0.79	0.08	1.53E-03	-0.06
Chlorine SC	0.60	0.58	0.06	1.28E-03	-0.05
Chemical factory	0.01	0.01	0.00	1.19E-05	-8.01E-04
Electricity (EU average)	0.04	0.04	0.01	1.06E-04	-4.24E-03
Natural gas SC	0.00	0.00	0.00	0.00	0.00
Heating (combustion)	0.00	0.00	0.00	0.00	0.00

Table S.12. LCA results (kg CO_2-eq) for the 1,5-pentanediamine (PDA) synthesis (stage C) within the production of 1kg of bio-PDI-T prepolymer.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land transformation	CO_2 uptake
TOTAL	9.69	9.60	0.50	0.02	-0.43
Direct emissions (process)	0.24	0.24	0.00	0.00	0.00
Water SC	4.18E-03	4.04E-03	4.70E-04	8.66E-06	-3.31E-04
Protein pea SC	-0.05	0.02	2.70E-04	2.29E-05	-0.07
Sodium chloride SC	0.01	0.01	6.83E-04	2.05E-05	-6.35E-04
Yeast extract SC	0.05	0.04	0.04	0.01	-0.04
Chemical factory	0.01	0.01	6.85E-04	1.19E-05	-8.01E-04
Sodium hydroxide SC	1.96	1.95	0.07	3.75E-03	-0.06
Enzymes SC	6.13E-04	1.31E-03	1.93E-04	1.09E-05	-9.00E-04
Potassium carbonate SC	0.14	0.14	0.01	2.03E-04	-0.01
Butanol SC	4.58	4.55	0.21	3.57E-03	-0.18
Ethanol SC	1.78	1.77	0.05	2.69E-04	-0.04
Natural gas SC	0.11	0.11	4.53E-04	3.55E-05	-3.93E-04
Electricity (EU average)	0.40	0.38	0.05	9.61E-04	-0.04
Heating (combustion)	0.38	0.38	0.00	0.00	0.00E+00
Biowaste treatment	0.08	0.01	0.08	2.90E-06	-2.27E-04
Solid waste treatment	0.00	0.00	0.00	0.00	0.00

Table S.13. LCA results (kg CO_2-eq) for the Pentamethylene diisocyanate (PDI) synthesis and oligomerization (stage E y F) within the production of 1kg of bio-PDI-T prepolymer.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land transformation	CO_2 uptake

TOTAL	8.34	8.11	0.83	0.02	-0.61
Direct emissions (process)	0.00	0.00	0.00	0.00	0.00
Water SC	1.50E-03	1.45E-03	1.68E-04	3.10E-06	-1.19E-04
Sodium hydroxide SC	0.67	0.66	0.02	1.27E-03	-0.02
Nitrogen SC	0.46	0.44	0.06	1.09E-03	-0.04
O-DCB SC	1.07	1.06	0.04	9.10E-04	-0.04
Chemical factory	0.01	0.01	6.85E-04	1.19E-05	-8.01E-04
Natural gas SC	0.17	0.17	7.46E-04	5.84E-05	-6.49E-04
Electricity (EU average)	5.35	5.15	0.70	0.01	-0.51
Heating (combustion)	0.62	0.62	0.00	0.00	0.00

Table S.14. LCA results (kg CO_2-eq) for the polyurethane synthesis from castor oil and PDI-T (stage G) within the production of 1kg of bio-PU resin.

Stage	GWP-100 (Total)	Fossil	Biogenic	Land transformation	CO_2 uptake
Total	22.80	22.33	2.90	0.88	-3.32
Direct emissions (process)	0.00	0.00	0.00	0.00	0.00
Castor oil SC	5.70	5.63	1.94	0.86	-2.73
Polyisocianate prepolymer SC	16.88	16.49	0.94	0.02	-0.57
Triethanolamine SC	0.05	0.05	1.01E-03	3.77E-05	-8.26E-04
Chemical factory	0.01	0.01	6.85E-04	1.19E-05	-8.01E-04
Natural gas SC	1.19E-03	1.19E-03	5.11E-06	4.00E-07	-4.44E-06
Electricity (EU average)	0.16	0.15	0.02	0.00	-0.02
Heating (combustion)	4.25E-03	4.25E-03	0.00	0.00	0.00

S.3. Process modelling results: Mass and energy balances

Table S.15. Inflow stream composition for the Molasses pretreatment (stage A)

Stream name	WATER	MOLASSES	H2SO4	NaOHaq	ActivCarb
Temperature (°C)	25	25	25	25	25
Pressure (bar)	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	9125.85	2607.39	462.16	9.20	243.91

Mass fraction (x_i)					
Water	1	0.2204	0.56	0.5	
Sucrose		0.357			
Glucose		0.039			
Fructose		0.059			
Galactose		0.0002			
Raffinose		0.0003			
Arabinose		0.0001			
CrudeProt		0.049			
Polysaccharides		0.016			
CarbAcid		0.062			
Ash		0.095			
Ion		0.052			
Solids		0.050			
Active carbon					1
H2SO4			0.440		
NaOH				0.5	

Table S.16. Outflow stream composition for the Molasses pretreatment (stage A)

Stream name	Out 1	Purif Molasses
Temperature (°C)	25	35
Pressure (bar)	1.01	1.01
Total flow (kg/h)	703.46	11,745.05
Mass fraction (x_i)		
Water		0.844
Glucose		0.050
Fructose		0.055
Galactose		4.44 E-5
Raffinose		6.66 E-5
Arabinose		2.22 E-5
CrudeProt		0.011
Polysaccharides		0.004
CarbAcid		0.014
Ash		0.021
Solids	0.185	
Active carbon	0.347	
Sulphate Ion	0.468	
Na2SO4		6.95 E-4
H2		3.43 E-4

Table S.17. Inflow stream composition for the L-lysine HCl synthesis (stage B)

Stream name	Purif Molasses	Culture med	Air ferment	HCl Sol	Air_2 drying

Temperature (°C)	35	25	25	25	25
Pressure (bar)	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	11,745.05	638.57	9,142.91	154.74	64.05
Mass fraction (x_i)					
Water	0.844	0.693		0.600	
Glucose	0.050				
Fructose	0.055				
Galactose	4.44 E-5				
Raffinose	6.66 E-5				
Arabinose	2.22 E-5				
CrudeProt	0.011				
Polysaccharides	0.004				
CarbAcid	0.014				
Ash	0.021				
Na2SO4	6.95 E-4				
H2	3.43 E-4				
Threonine		0.010			
NH4OH		0.297			
HCl				0.400	
O2			0.233		0.233
N2			0.767		0.767

Table S.18. Outflow stream composition for the L-lysine HCl synthesis (stage B)

Stream name	Ferm Gases	Wet biomass	Steam out	Purge	Air dry out	Sugar purg	L-lysine HCl
Temperature (°C)	30	30	110	20	25	55	45
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	1.01

Total flow (kg/h)	9,410.67	124.94	10,845.26	192.01	65.51	792.26	314.67
Mass fraction (x_i)							
Water		0.020	0.998	0.520	0.022		0.015
Glucose						0.114	
Fructose						0.124	
Galactose						6.58E-04	
Raffinose						9.87E-04	
Arabinose						3.29E-04	
CrudeProt						0.161	
Polysaccharides						0.053	
CarbAcid						0.204	
Ash						0.313	
Biomass		0.980					
O2	0.181		8.20E-06		0.228	3.32E-05	
N2	0.746		4.09E-06		0.750	1.66E-05	
NH3			1.33E-04				
H2			4.03E-04			0.005	
CO2	0.073		0.001			0.005	
Threonine						0.004	
NH4OH						0.006	
Na2SO4						0.010	
Lysine				0.48			
Lysine-HCl							0.985

Table S.19. Inflow and outflow stream composition for the Phosgene synthesis (stage D)

	Inflow streams		Outflow streams	
Stream name	COin	Clin	Purge	Phosgene_out
Temperature (°C)	25	25	-15	-15
Pressure (bar)	1.01	1.01	2.00	2
Total flow (kg/h)	94.43	238.90	0.35	332.98

Mass fraction (x_i)				
CO	1.000		0.398	2.12E-04
Cl2		1.000	5.26E-05	
CCl2O			0.602	1.000
CrudeProt		0.011		
		0.004		
Polysaccharides				
CarbAcid		0.014		
Ash		0.021		
Solids	0.185			
Active carbon	0.347			
Sulphate Ion	0.468			
Na2SO4		6.95 E-4		
H2		3.43 E-4		

Table S.20. Inflow stream composition for the 1,5-pentanediamine (PDA) synthesis (stage C)

Stream name	L-lysine HCl	Culture med	Bacteria inocul	Lys HCl initiator	Air ferm	EthanWa	Buffer in1
Temperature (°C)	45	25	25	25	25	25	25
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	314.67	993.37	0.48	2.00	12.04	1113.61	678.78
Mass fraction (x_i)							
Water	0.015	0.975				0.700	0.991
Lysine-HCl	0.985			1.000			
Peptone		0.010					
NaCl		0.010					
Yeast extract		0.005					
NaOH							
O2					0.233		
N2					0.767		
Pyr_phos							
KH2PO4							0.009
Ecoli			1.000				
Butanol							
Ethanol						0.300	

Table S.20 (cont.). Inflow stream composition for the 1,5-pentanediamine (PDA) synthesis (stage C)

Stream name	Coenzyme	Buffer in2	NaOH	MU butanol
Temperature (°C)	25	25	25	25
Pressure (bar)	1.01	1.01	1.01	1.01
Total flow (kg/h)	0.03	422.26	344.71	282.00
Mass fraction (x_i)				

Water		0.991		
Lysine-HCl				
Peptone				
NaCl				
Yeast extract				
NaOH			1.000	
O2				
N2				
Pyr_phos	1.000			
KH2PO4		0.009		
Ecoli				
Butanol				1.000
Ethanol				

Table S.21. Outflow stream composition for the 1,5-pentanediamine (PDA) synthesis (stage C)

Stream name	Out7	Out8	Out9	Out10	Out11	Out12
Temperature (°C)	37	37	4	37	37	55
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	12.04	992.45	1113.61	54.36	2.54	37.59
Mass fraction (x_i)						
Water		0.976	0.7			
Peptone		0.008				
NaCl		0.010				0.263
Yeast extract		0.004				
NaOH						0.737
O2	0.212					
N2	0.767					
Lysine						
CO2	0.021			1		
Pyr_phos		0.002				
KH2PO4						
Lysine HCl						
Butanol						
Ethanol			0.3			
Ecoli_p					1	
PDA-HCl						
PDA						

Table S.21 (cont.). Outflow stream composition for the 1,5-pentanediamine (PDA) synthesis (stage C)

Stream name	AccumTank2	Out 13	Aq emiss2	Out 15	Cadav_out
Temperature (°C)	4	55	30	30	30
Pressure (bar)	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	172.46	1,307.03	53.21	263.89	154.77
Mass fraction (x_i)					
Water	0.986	0.663	0.939	0.151	

Peptone					
NaCl		0.068			
Yeast extract					
NaOH		0.191			
O2					
N2					
Lysine		0.016			
CO2		0.011			
Pyr_phos		2.37E-05			
KH2PO4	0.009	0.006			
Lysine HCl		0.002			
Butanol		0.043	0.061	0.843	3.60 E-4
Ethanol					
Ecoli_p	0.005				
PDA-HCl					
PDA				0.006	1.000

Table S.22. Inflow stream composition for the Pentamethylene diisocyanate (PDI) synthesis (stage E)

Stream name	Cadav_out	Phosgene	oDCB	N2in	NaOHaq	Wat for HCl
Temperature (°C)	30	-15	25	25	25	25
Pressure (bar)	1.01	2	1.01	1.01	1.01	1.01
Total flow (kg/h)	154.77	332.98	115.96	499.40	176.83	858.61
Mass fraction (x_i)						
Water		2.12E-04			0.500	1.000
CO						
CCl2O		1.000				
NaOH					0.500	
N2				1.000		
Butanol	3.60 E-4					
o-DCB			1.000			
Trim cat						
PDA	1.000					

Table S.23. Outflow stream composition for the Pentamethylene diisocyanate (PDI) synthesis (stage E)

Stream name	Out 16	Out 17	Out20	Out18	Out19	PDI out
Temperature (°C)						
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Total flow (kg/h)	35.31	998.38	508.06	248.70	116.66	231.44
Mass fraction						

(x_i)						
Water		0.860		0.499	2.46E-04	
CO					6.06E-04	
CCl2O	1.000					
NaCl				0.462		
NaOH				0.039	0.500	
HCl			0.017			
N2		0.005	0.983		0.001	
Butanol					4.78E-04	
o-DCB		0.135			0.984	0.005
PDA					0.013	
PDI					7.93E-04	0.995

Table S.24. Inflow stream composition for the Pentamethylene diisocyanate (PDI) oligomerization and PU polymerization (stages F y G)

Stream name	PDI out	TMR-catal	Steam in	Castor oil	TEDA
Temperature (ºC)	25	25	145	25	25
Pressure (bar)	1.01	1.01	3.21	1.01	1.01
Total flow (kg/h)	231.44	0.13	2.57	318.17	9.55
Mass fraction (x_i)					
Water		0.700	1.000		
o-DCB	0.005				

TMR		1.000		
PDI	0.995			
Castor oil			1.000	
TEDA				1.000

Table S.25. Outflow stream composition for the Pentamethylene diisocyanate (PDI) oligomerization and PU polymerization (stages F y G)

Stream name	Out21	Conden out	PU out
Temperature (°C)	25	145	25
Pressure (bar)	1.01	3.21	1.01
Total flow (kg/h)	4.50	2.57	554.79
Mass fraction (x_i)			
Water		1.000	
o-DCB	0.256		
TMR			
PDI	0.744		
PU-resin			1.000
TEDA			

Table S.26. Heat flows within the whole bio-PU production process.

Subprocess	Unit name	Heat flow (kW)	Tin (°C)	Tout (°C)	Supplied Internally
A. Molasses pretreatment	Tank1	513.867	20	60	Yes
	HX1	831.879	60	121	
	HX2	-1172.809	121	20	
B. Lysine-HCl synthesis	HX3	0	-	-	
	HX4	7.415	20	30	
	Evapor1	7607.804	30	100	
	HX5	-118.543	100	20	
	HX6	1.171	20	86	Yes

D. Phosgene synthesis	HX7	-2.133	128.04	50	
	HX8	-2.243	118.89	50	
	React1	-106.923	50	50	
	HX9	-26.599	48	-15	Ammonia ref cycle*
	HX10	0.249	16.7	50	Yes
C. PDA synthesis	HX11	0	37	37	
	HX12	-0.066	56.664	37	
	HX13	-409.805	20	4	Ammonia ref cycle*
	HX14	10.061	20	37	Yes
	HX15	14.547	20	37	Yes
	HX16	76.613	37	80	Yes
	HX17	-44.543	80	55	
	HX18	22.757	30	55	Yes
	HX19	49.302	55	90	
	Cond_DC1	-362.089		92	
	Evap_DC1	197.759		178	
	HX20	-12.935	178	30	
	HX21	-78.485	92	30	
	HX22	116.495	20	121	Yes (partially)
	HX23	-96.887	121	37	
E. PDI synthesis	HX24	14.941	20	60	Yes
	HX25	10.924	20	60	Yes
	HX26	-208.939	292.7	150	
	React3	64.791	60	150	
	HX27	111.479	-52.873	20	Yes
	Cond_DC2	-315.863		-153	N_2 ref cycle**
	Evap_DC2	12.006		7.3	Yes
	HX28	1.141	20	20	Yes
	HX29	0	7.3	20	
	Cond_DC3	-355.426		-84	N_2 ref cycle***
	Evap_DC3	406.867		147	
	HX30	0	-	-	
	HX31	-13.126	-86.8	20	
	HX32	-42.618	146.5	20	

F. PDI oligomerization	HX33	8.524	20	80	Yes
	HX34	11.701	80	129	
	Dist TF	1.47	129.1	160	
	Cond_FD	-9.258	129.1	129	
	HX35	-9.071	129.1	20	
	HX36	-4.393	160	20	
G. PU polymerization	HX37	8.114	20	50	Yes
	React5	-25.347	50	50	

* Coefficient of performance (COP) of 1.29 [26]

** Coefficient of performance (COP) of 0.15 (T = 100 K) [27]
*** Coefficient of performance (COP) of 0.15 (T = 150 K) [27]

Table S.27. Power consumption by unit within the whole bio-PU production process.

Subprocess	Unit name	Power consumption (kW)
A. Molasses pretreatment	Pump1	7.833
B. Lysine-HCl synthesis	Blower1	92.66
	Blower2	1.352
D. Phosgene synthesis	Comp1	3.465
	Comp2	3.415
	HX9	20.62
	Comp3	0.212
C. PDA synthesis	Blower3	0.142
	HX13	15.88
	Tank4	60
	Tank5	60
	React2	75.3
	Tank6	39.467
E. PDI synthesis	Pump2	0.081
	Pump3	0.178
	Pump4	0.343
	Comp4 (2 stages)	462.51
	Exp1	-115.593
	Pump5	0.036
	Cond_DC2	2,105.75
	Cond_DC3	888.57
F. PDI oligomerization	React4	0.584
	Distillation TF	0.592
	Pump6	0.008
	Vacuum pump	15.822
	Pump7	0.003
G. PU polymerization	React5	0.12
	Oven	240

Table S.28. Heat requirements and heat integration. Saturated steam at 1 bar produced at the evaporator is used as the heating process stream.

Unit Operation	Heat transfer (kW)	Temperature in (ºC)	Temperature out (ºC)	Internal supply
Tank1	513.9	20	60	Yes
HX1	831.9	60	121	Partially (33%)
HX2	-1172.8	121	20	
HX4	7.4	20	30	Yes
Evapor1	7607.8	30	100	
HX5	-118.5	100	20	

HX6	1.2	20	85	Yes
HX7	-2.1	128	50	
HX8	-2.2	119	50	
React1	-106.9	50	50	
HX10	0.2	17	50	Yes
HX12	-0.1	57	37	
HX13	-409.8	20	4	
HX14	10.1	20	37	Yes
HX15	14.5	20	37	Yes
HX16	76.6	37	80	Yes
HX17	-44.5	80	55	
HX18	22.8	30	55	Yes
HX19	49.3	55	90	
Cond_DC1	-362.1		92	
Evap_DC1	197.8		178	
HX20	-12.9	178	30	
HX21	-78.5	92	30	
HX22	116.5	20	121	Partially (33%)
HX23	-96.9	121	37	
HX24	14.9	20	60	Yes
HX25	10.9	20	60	Yes
HX26	-208.9	293	150	
React3	64.8	60	150	
HX27	111.5	-53	20	Yes
Cond_DC2	-315.9		-153	
Evap_DC2	12.0		7	Yes
HX28	1.1	20	20	Yes
Cond_DC3	-355.4		-84	
Evap_DC3	406.9		147	
HX31	-13.1	-87	20	
HX32	-42.6	147	20	
HX33	8.5	20	80	Yes
HX34	11.7	80	129	
Dist_TF	1.5	129	160	
Cond_FD	-9.3	129	129	
HX35	-9.1	129	20	
HX36	-4.4	160	20	
HX37	8.1	20	50	Yes
React5	-25.3	50	50	
Total heat demand (kW)	10,169.7		Total Heat internally supplied (kW)	1,148.3

S.4. Assumptions

A. Molasses pretreatment

- Sugar loss in pretreatment: 2%
- Sucrose conversion in hydrolysis: 100% (pH = 2)
- Conversion of ions and neutralization: 100%
- Dilution in water: 3.5 kg water/kg molasses; heat to 60°C to reduce viscosity

- Filter removal efficiency: 100%

B. Lysine-HCl synthesis

- Fermenter volume: 200 m^3
- Continuous production using multiple equipment units
- NH_4OH as nitrogen source
- Yield: 0.17 g L-lysine/g glucose (experimental)
- Fermentation time: 48 hours (experimental)
- Sugar conversion: 52.4% (calculated from yield experimental data). Remaining sugar only separated by ultrafiltration and recycled
- Evaporation at ambient temperature (vacuum conditions for evaporation were estimated to save 10% energy but increases cost and worsens heat transfer)
- Supersaturation lysine solution: 40%
- Crystallization yield: 35%

C. PDA synthesis

- Modified E. coli fermentation: 12 hours
- Cell permeabilization: 0.5 hours at 4°C (100% yield)
- Filter efficiency: 100%
- Deprotonation time: 5 hours (100% conversion)
- Butanol absorption yield based on solubility (equilibrium)
- Distillation separation based on process modeling
- Accumulation tank after cell permeation for continuous downstream flow

D. Phosgene synthesis

- On-demand production
- Operating conditions: 50°C, 3 bar
- Excess CO; 100% conversion of limiting reactant
- CO sourced from petrol, Cl_2 purchased
- Cryogenic separation with NH_3 refrigeration
- Phosgene in purge neutralized with NaOH

E. PDI synthesis

- Liquid phosgenation with dichlorobenzene as solvent
- Phosgene to PDA molar ratio = 4:1

- Batch process, continuous production using multiple equipment
- Two-step phosgenation: cold (50°C) and hot (150°C) at 10 bar
- Nitrogen flush, recycled
- Phosgene recovery from volatiles: distillation (Aspen Plus simulation)
- PDI recovery from DCB: distillation (Aspen Plus simulation)
- Absorption: liquid-liquid equilibrium, DCB and PDA recycled

F. PDI oligomerization

- Oligomerization reaction time: 2 hours
- Product distribution (experimental data):
    - x_PDIout = 0.25
    - x_PDITout = 0.47
    - x_PDIPout = 0.20
    - x_PDIHout = 0.08
- Thin film distillation for PDI recovery and recycling (3% PDI in final PDI-T product)
- Thermodynamic properties of PDI: modeled using Aspen Plus

G. PU polymerization

- Type: Bulk polymerization (one-shot method)
- NCO:OH molar ratio = 1.5:1
- Prepolymer reaction at 50°C for 10 min in a CSTR with refrigeration
- Catalyst: Triethylenediamine (3% mass ratio)
- Curing reaction in mold at 80°C (electric oven, 30 kW)

General Assumptions for the LCA

- Entire process performed in the same plant
- Raw materials transported to the plant
- Heat integration performed where possible
- Plant lifetime: 25 years with an 80% operational factor
- Reused materials for multiple cycles (e.g., activated carbon, DCB solvent, butanol, ethanol, nitrogen) are purged in a 10-20% ratio downstream to prevent degradation.
- Heating provided by natural gas boilers (efficiency: 0.72)

- CO_2 emissions are vented
- Electricity sourced from the grid (EU average environmental impact)
- Three cryogenic refrigeration cycles:
    - Ammonia, HX9 and HX13. T refrigerant = 240 K (COP = 1.29)
    - Nitrogen, DC2 condenser: T refrigerant = 90 K (COP = 0.15)
    - Nitrogen, DC3 condenser: T refrigerant = 130 K (COP = 0.4)

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