

Chemical Recycling of Post-Industrial Plastic Waste: Life Cycle Assessment of a Pre-Commercial Chemical Recycling Process: *Supplementary Information*

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A. Life cycle inventory of the chemical recycling process for 1 kg of total obtained products

Table 1. Life cycle inventory of the chemical recycling process for 1 kg of total obtained products

Input and output flows based on 1 kg of TOP		Feedstock 1	Feedstock 2	Unit
Inputs	Feedstock	1.15	1.46	kg
	Catalyst	22.63	26.07	g
	Electricity Recycling Process	2.35	2.06	kWh
	Steam hydrogenation and separation	0.30	0.26	kWh
	Electricity hydrogenation and separation	0.18	0.12	kWh
	Hydrogen	52.21	34.94	g
Outputs	Paraffines/Olefines	0.86	0.59	kg
	of which Naphtha	0.17	0.09	kg
	of which Diesel	0.45	0.34	kg
	of which Heavy Oil	0.24	0.16	kg
	Wastewater	0.05	0.04	kg
	Aromatics	0.14	0.41	kg
	of which caprolactam	0.13	0.32	kg
	of which BTEX	0.01	0.09	kg
	Particles < 2 mm	-	0.02	g
	Ferrous metals	1.26	1.17	g
	Non-ferrous metals	0.00	0.29	g
	Residue	0.00	0.22	kg
	Process gas	0.12	0.21	kg

B. Life cycle inventory of the incineration process derived by the Municipal Solid Waste Incineration (MSWI) model by Doka

The incineration process is calculated using the Doka model [1]. The conversion tables used and the resulting life cycle inventory are shown in the tables below.

Table 2. MSWI conversion table for the incineration process [1]

Element	Slag	Boiler Ash	ESP Ash	Scrubber Sludge	Water Emissions	Air Emissions
H2O	0	0	0	0	0	1000
O	69.8	2.04	10.2	1.02	0	917
H	0	0	0	0	0	1000
C	7.55	0	3.44	0.0101	0.0101	989
S	554	0	298	74.6	71.4	2.13
N	10	0	0	0	1	989
P	880	25	94	0	0	1
B	384	0	166	180	151	120
Cl	71.3	0	13	6.48	909	0.0108
Br	110	10	877	0	0	3
F	615	0	308	21	56	0.5
I	71.3	0	13	6.48	909	0.0108
Ag	615	5.32	274	106	0.0729	0.013
As	550	30	381	39	0.1	1.02E-05
Ba	887	22	90	0	0	1
Cd	3.27	0	369	627	0.441	0.0551
Co	850	10	120	20	0.01	3.18E-05
Cr	455	31.9	446	63.7	3.19	7.39E-05
Cu	801	0	185	14.8	0	0.00738
Hg	5.74	2.09	366	615	10.5	3.45E-05
Mn	860	10	120	10	0.01	5.45E-06
Mo	867	21	110	0	0	2
Ni	901	35.5	63.5	0	0	4.32E-05
Pb	66.4	0	848	85.4	0.0186	0.0371
Sb	16.1	18.2	822	144	0.182	3.89E-06
Se	80.3	130	719	70.7	0.118	5.03E-06
Sn	496	19.9	451	31.8	0.0133	1.33
V	890	10	90	10	0.01	0.1
Zn	3.29	0	817	180	0.163	0.0163
Be	696	0	294	9	0	1
Sc	999	0	0	0.5	0	0.5
Sr	999	0	0	0.9	0	0.1
Ti	999	0	0	0	0	1
Tl	348	0	650	1	0	1
W	751	0	249	0	0	0
Si	919	25.6	53.5	0	0	2.33
Fe	899	0	93.5	6.68	0.334	0.0334
Ca	862	36.7	100	0	0	1.67
Al	853	35.9	109	0	0	1.56
K	668	47.2	281	0	0	3.01
Mg	917	20.7	60.6	0	0	1.38
Na	614	94.1	282	0	0	9.41

Table 3. Life cycle inventory of the incineration process

Input/Output	Name	Feedstock A	Feedstock B	Unit
Input	Feedstock	1	1	kg
	Electricity	127.3	127.3	Wh
	Heat	134.81	134.81	Wh
	Air	15.2	15.0	kg
Outputs	Electricity	1062.1	1093.9	Wh
	Heat	3363.2	3464.2	Wh
	Slag component			
	C	0.008383456	0.008851061	kg
	SO3	-	0.000923312	kg
	NO3	0.001824981	0.000595928	kg
	P2O5	0.000252104	-	kg
	TiO2	0.000309278	-	kg
	SiO2	0.002111805	-	kg
	Fe2O3	0.000382603	-	kg
	CaO	0.004406353	-	kg
	Cl	-	0.000176393	kg
	F	-	0.00018813	kg
	Al2O3	0.000757545	-	kg
	Air Emissions Component			
	H2O	1.120944327	1.037025563	kg
	CO2	2.761886335	2.915936436	kg
	SO2	0	1.69626E-06	kg
	NO2	0.133885253	0.043718773	kg
	P	1.10199E-07	-	kg
	SiO2	2.30368E-06	-	kg
	Fe2O3	8.94365E-09	-	kg
	CaO	5.26299E-06	-	kg
	Al2O3	6.26591E-07	-	kg
	HCl	-	2.15819E-08	kg
	HF	-	1.04932E-07	kg
	Water Emissions			
	TOC	7.69747E-06	8.12681E-06	kg
SO4	-	8.52562E-05	kg	
NO3 (-)	0.000182439	5.95736E-05	kg	
Fe ion	8.94365E-08	-	kg	

C. Background System of the Life Cycle Assessment

Table 4. Background Data for the input flows used in the life cycle assessment

Input flow	Unit	Provider	Source
Heat from steam	kWh	market for heat, from steam, in chemical industry heat, from steam, in chemical industry Cutoff, S - RER	Ecoinvent
Electricity	kWh	market for electricity, low voltage electricity, low voltage Cutoff, S - DE	Ecoinvent
Hydrogen, gaseous	kg	market for hydrogen, gaseous hydrogen, gaseous Cutoff, S - GLO	Ecoinvent
Catalyst	kg	market for zeolite, powder zeolite, powder Cutoff, S - GLO	Ecoinvent

Table 5. Background Data for the product flows used in the life cycle assessment

Product flow	Unit	Provider	Source
Naphtha	kg	naphtha production, petroleum refinery operation naphtha Cutoff, S - Europe without Switzerland	Ecoinvent
Diesel	kg	diesel production, petroleum refinery operation diesel Cutoff, S - Europe without Switzerland	Ecoinvent
Heavy fuel oil	kg	heavy fuel oil production, petroleum refinery operation heavy fuel oil Cutoff, S - Europe without Switzerland	Ecoinvent
Reformate	kg	reformate production, petroleum refinery operation reformate Cutoff, S - Europe without Switzerland	Ecoinvent
Caprolactam	kg	caprolactam, production mix - DE	carbonminds
Ferrous metals	kg	market for ferrous metal, in mixed metal scrap ferrous metal, in mixed metal scrap Cutoff, S - Europe without Switzerland	Ecoinvent
Nonferrous metals	kg	market for aluminum, in mixed metal scrap aluminum, in mixed metal scrap Cutoff, S - Europe without Switzerland	Ecoinvent

Table 6. Background Data for the waste flows treated in the life cycle assessment

Waste flow	Unit	Treatment method	Source
Particles < 2 mm	kg	treatment of wastewater, average, wastewater treatment wastewater, average Cutoff, S - Europe without Switzerland	Ecoinvent
Wastewater	kg	treatment of wastewater, average, wastewater treatment wastewater, average Cutoff, S - Europe without Switzerland	Ecoinvent
Solid residue	kg	treatment of refinery sludge, hazardous waste incineration, with energy recovery refinery sludge Cutoff, S - Europe without Switzerland	Ecoinvent
Process gas	kg	self-defined based on: treatment of blast furnace gas, in power plant electricity, high voltage Cutoff, S	Ecoinvent
Incineration sludge	kg	treatment of bottom ash, MSWI-WWT, WW, average, slag compartment bottom ash, MSWI-WWT, WW, average Cutoff, S - Europe without Switzerland	Ecoinvent

D. Development of the ASPEN Plus Downstream Sequence

A two-dimensional gas chromatography measurement of each product flow was conducted. For the paraffin/olefin-rich fraction, the analysis successfully identified and quantified 93.92% of the total components for Feedstock A and 94.57% for Feedstock B. The results were then clustered into categories such as paraffins, olefins, alkylbenzenes, and significant substances that didn't fit in any category. This clustering process considered 94.31% of the identified substances, encompassing 74 individual components for Feedstock A, and 97.47% of Feedstock B, also encompassing 74 individual components. To reduce the number of components for the simulation process, the mixture of substances was reduced by eliminating all compounds with a concentration of less than 0,5%. This reduction resulted in a final set of 47 individual compounds for Feedstock A and 49 individual compounds for Feedstock B, which were then used in the subsequent simulation.

Distillation

The substance data model was derived using the Method Assistant and set to the Peng-Robinson equation of state (Refining → an Atmospheric Crude Tower → PENG-ROB equation of state). Although other methods were available, Peng-Robinson was chosen based on previous publications [2, 3]. A RadFrac column was designed with 25 stages and a reflux ratio of 3. The reboiler duty is 27.35 kW at an input flow of 100 kg/h. The column has three output flows: head distillate (Naphtha with a boiling temperature < 200 °C), bottom product (Heavy Oil > 360 °C), and at stage 15 (Diesel 200 – 360 °C) [4, 5]. Parameter adjustments were made as follows:

1. Reflux ratio and reboiler duty were adjusted for optimal separation between Naphtha and Diesel. The goal was to ensure that the first compound with a boiling point above 180 °C ($C_{13}H_{28}$) was minimally present in the Naphtha fraction (> 2%) while maintaining low energy consumption in the reboiler.
2. The number of stages and the amount of diesel output were adjusted to achieve optimal separation between Diesel and Heavy Oil. The first compound with a boiling point below 360 °C ($C_{21}H_{44}$) should be entirely in the Diesel fraction, while the first compound with a boiling point above 360 °C ($C_{22}H_{44}$) should be entirely in the Heavy Oil fraction.
3. The adjustments were made iteratively to ensure that the conditions from the first step were not compromised.

Hydrogenation

The hydrogenation flow sheet was designed as follows: the oil was first pumped into the reactor at 50 bar, and the hydrogen was compressed to 50 bar and led into the reactor. The reactor itself was modelled as a stoichiometric "RSTOIC" reactor. Complete conversion of all alkenes to alkanes was assumed to give the highest possible energy requirement. The amount of hydrogen required was taken from the literature as 500 m³ of hydrogen per m³ of oil [6]. To determine the amount of hydrogen, the density of the oil was calculated using Aspen Plus. This density-to-hydrogen ratio was then used to determine the amount of hydrogen required. Reaction conditions were set at 50 bar and 350°C as reported in the literature [4, 6–8]. It was assumed that the energy required for pumping and compression would be provided by electricity and that the energy required to maintain the reaction conditions in the reactor would be provided by steam. The amount of catalyst used for hydrogenation has been neglected in the inventory. To justify this assumption, we conducted preliminary calculations showing the hydrogenation to not exceed 10% of the total process emissions. Publications as [9] have pointed out that the catalyst could impact from 1% to 5% of hydrogenation GWP and therefore would never contribute >0.5% to the total process emissions and be cut off in the LCIA (cut off < 1%).

E. Life Cycle Assessment results based on each product obtained

Table 7. Life cycle impact assessment results of the recycling process based on 1kg of each product for the impact categories Global Warming Potential (GWP), Marine (MEP) and Freshwater (FEP) Eutrophication Potential, Terrestrial Acidification Potential (TAP) and Fossil Fuel Depletion potential (FFDP)

	GWP [kg CO2-eq]		MEP [kg N-eq*10000]		FEP [kg P-eq*10000]		TAP [kg SO2-eq*1000]		FFDP [kg Oil-eq]	
	Feedstock A	Feedstock B	Feedstock A	Feedstock B	Feedstock A	Feedstock B	Feedstock A	Feedstock B	Feedstock A	Feedstock B
LCA results for 1 kg of Caprolactam										
Chemical recycling process	9.13	3.28	7.68	2.82	119.28	41.96	19.45	7.17	2.25	0.81
Product upgrading	2.41	0.61	1.37	0.30	10.39	2.81	6.14	1.38	1.47	0.29
Waste treatment	0.90	2.23	0.00	0.35	0.00	1.14	0.00	2.00	0.00	0.41
Substitution caprolactam										
Substitution Naphtha	-1.05	-0.21	-1.23	-0.24	-0.53	-0.11	-2.34	-0.46	-1.57	-0.31
Substitution Diesel	-3.14	-0.96	-3.27	-1.00	-1.44	-0.44	-8.66	-2.63	-4.16	-1.27
Substitution Heavy Oil	-1.37	-0.37	-1.58	-0.42	-0.68	-0.18	-3.04	-0.81	-2.03	-0.54
Substitution Reformat	0.00	-0.26	-0.10	-0.24	0.00	-0.10	0.00	-0.84	-0.12	-0.31
LCA results for 1 kg of Naphtha										
Chemical recycling process	6.82	12.37	5.74	10.64	89.09	158.03	14.53	27.02	1.68	3.06
Product upgrading	1.80	2.31	1.02	1.12	7.76	10.57	4.58	5.19	1.10	1.08
Waste treatment	0.67	8.39	0.00	1.33	0.00	4.28	0.00	7.55	0.00	1.54
Substitution Caprolactam	-6.37	-32.14	-1.67	-8.42	-8.74	-43.18	-19.23	-96.85	-2.48	-12.53
Substitution Naphtha										
Substitution Diesel	-2.34	-3.60	-2.44	-3.75	-1.08	-1.66	-6.47	-9.92	-3.11	-4.78
Substitution Heavy Oil	-1.02	-1.39	-1.18	-1.60	-0.50	-0.68	-2.27	-3.03	-1.52	-2.05
Substitution Reformat	0.00	-1.00	-0.07	-0.91	0.00	-0.39	0.00	-3.15	-0.09	-1.17
LCA results for 1 kg of Diesel										
Chemical recycling process	2.62	3.09	2.21	2.66	34.27	39.51	5.59	6.75	0.65	0.76
Product upgrading	0.69	0.58	0.39	0.28	2.98	2.64	1.76	1.30	0.42	0.27
Waste treatment	0.26	2.10	0.00	0.33	0.00	1.07	0.00	1.89	0.00	0.38
Substitution Caprolactam	-2.45	-8.03	-0.64	-2.11	-3.36	-10.79	-7.40	-24.21	-0.96	-3.13
Substitution Naphtha	-0.30	-0.20	-0.35	-0.23	-0.15	-0.10	-0.67	-0.44	-0.45	-0.29
Substitution Diesel										
Substitution Heavy Oil	-0.39	-0.35	-0.45	-0.40	-0.19	-0.17	-0.87	-0.76	-0.58	-0.51
Substitution Reformat	0.00	-0.25	-0.03	-0.23	0.00	-0.10	0.00	-0.79	-0.04	-0.29
LCA results for 1 kg of Heavy Oil										
Chemical recycling process	4.91	6.52	4.13	5.61	64.09	83.32	10.45	14.25	1.21	1.61
Product upgrading	1.29	1.22	0.73	0.59	5.58	5.58	3.30	2.74	0.79	0.57
Waste treatment	0.48	4.42	0.00	0.70	0.00	2.25	0.00	3.98	0.00	0.81
Substitution Caprolactam	-4.59	-16.95	-1.20	-4.44	-6.29	-22.77	-13.83	-51.07	-1.79	-6.61
Substitution Naphtha	-0.56	-0.41	-0.66	-0.48	-0.29	-0.21	-1.26	-0.92	-0.85	-0.62
Substitution Diesel	-1.69	-1.90	-1.75	-1.98	-0.77	-0.87	-4.65	-5.23	-2.23	-2.52
Substitution Heavy Oil										
Substitution Reformat	0.00	-0.53	-0.05	-0.48	0.00	-0.21	0.00	-1.66	-0.07	-0.61

F. Life cycle impact assessment results considering the development of the electricity mix

Table 8. Life cycle impact assessment results considering the development of the electricity mix. 2030 represents a share of renewables of 80 % while 2038 represents full use of renewables

Impact category	Feedstock A		Feedstock B		Unit
	2030	2038	2030	2038	
GWP	1.06E+00	6.48E-01	1.49E+00	1.14E+00	kg CO ₂ -eq
FFDP	3.23E-01	2.14E-01	3.44E-01	2.46E-01	kg oil-Eq
TAP	2.29E-03	2.00E-03	2.43E-03	2.26E-03	kg SO ₂ -eq
FEP	7.44E-04	1.20E-04	6.93E-04	1.48E-04	kg P-eq
MEP	6.17E-05	2.35E-05	6.20E-05	2.90E-05	kg N-eq

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