Supplementary Information (SI) for Green Chemistry.

***SUPPLEMENTARY MATERIAL:** SUPERSTRUCTURE OPTIMIZATION FOR MANAGEMENT OF LOW-DENSITY POLYETHYLENE PLASTIC WASTE.*

Borja Hernández, D.G. Vlachos, Marianthi G. Ierapetritou

Department of Chemical and Biomolecular Engineering and Center for Plastics Innovation, University of Delaware, 221 Academy Street, Suite 250, Newark, Delaware 19716, USA.

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S-1. DESCRIPTION OF MODELS FOR THE TECHNOLOGIES

S-1.1 Landfill

The first and simplest option in the superstructure is sending the plastic to a landfill. The cost for this case is assumed to be the same as the one reported for Municipal Solid Waste (MSW). The average cost in US per ton of MSW is \$53/ton.[1] The GWP of the landfill is assumed as the one of "Treatment of waste plastic mixture, unsanitary landfill, moist infiltration class (300 mm)".

S-1.2 Incineration

Incineration is composed of three sections, see Figure S-1. First, the plastic is cut with a shredder then is burnt in a furnace which is used for generating steam and producing power in the last section. The operating cost in the shredder is determined as a function of the power consumed based on Larrain et al.[2] The following linear model, Eq. (S-1), is determined based on the data of the paper.

$$W_{shredder}\left(\frac{kWh}{s}\right) = 3.482{\cdot}10^{-2} f_{LDPE}\left(\frac{kg}{s}\right) \tag{S-1}$$

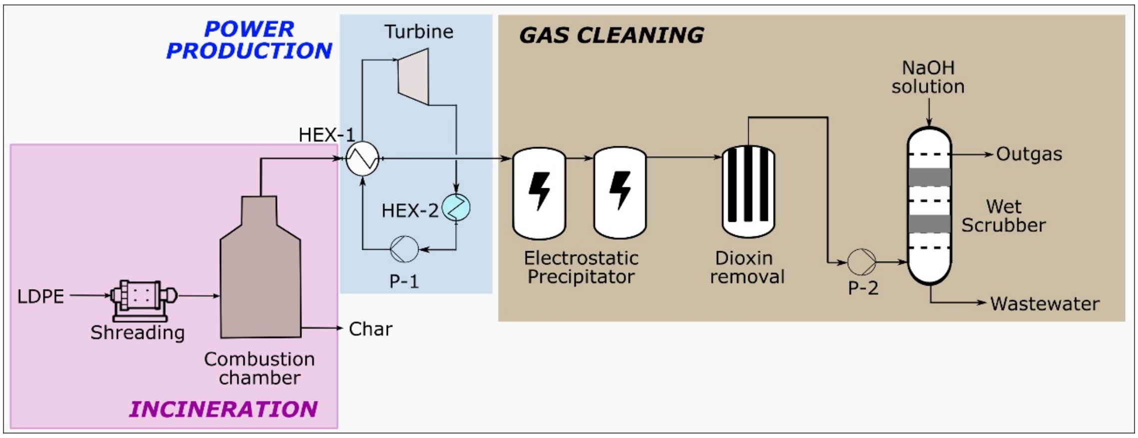

Figure S-1. Process for the production of power.

The energy produced in the incineration is determined as in Bora et al.[3] with the energy efficiency in the production of power from MSW ($\eta_{incin} = 30\%$) based on the process presented in Pavlas,[4] see Eq. (S-2). The total energy input in the incineration, E$_{in}$, is determined from the energy balance of the combustion reaction, Eq. (S-3). By performing the mass and energy balances, the energy produced per kg of LDPE is estimated as presented in Eq. (S-4).

$$W_{prod\ incin} = E_{in}{\cdot}\eta_{incin} \tag{S-2}$$

$$-CH_2- \ + \frac{3}{2}O_2 \rightarrow CO_2 + H_2O \tag{S-3}$$

$$W_{prod\ incin}\left(\frac{kWh}{s}\right) = 12531.8{\cdot}f_{LDPE}\left(\frac{kg}{s}\right) \tag{S-4}$$

The cost of units is determined as the summation of the shredder, the furnace, the heat exchanger used to boil the water, and the turbine. All the costs are determined with the cost estimator tool of the book of Peters et al.[5] The final CAPEX obtained for the process is implemented as the piecewise linear model generated from Eq. (S-5).

$$CAPEX\left(\frac{\$}{s}\right) = 0.09013 \cdot f_{LDPE}{}^{0.8257} \qquad \text{(S-5)}$$

S-1.3 Pretreatment for plastic recycling

Mass and energy balances of the pretreatment are performed following the process described in Larrain et al.,[2] see Figure S-2. The OPEX is determined to include the utilities and chemicals used for cleaning the plastics. A summary of the utilities and chemicals required per kg of LDPE treated is given in Table S-1, taken from Larrain et al.[2]

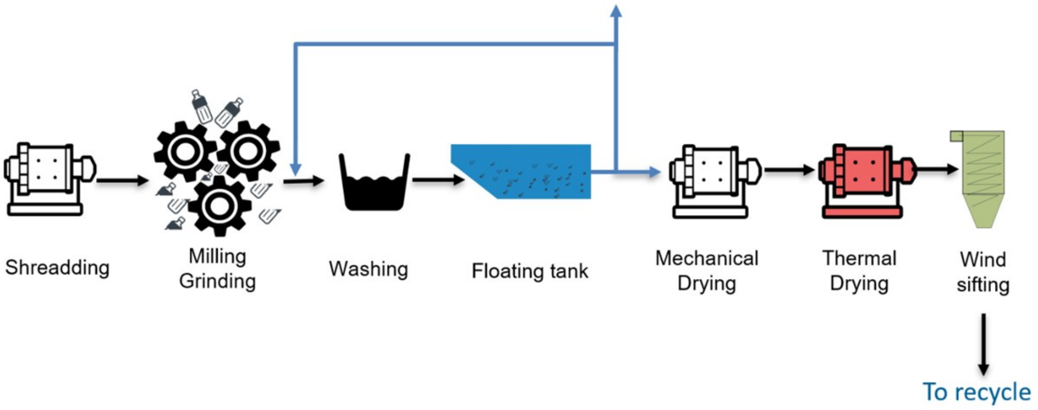

Figure S-2. Pre-processing of the plastics.

Table S-1. Summary of resources required in the plastic treatment and sorting plant.

Utility / Raw material	Consumption	Price	Cost ($\$/kg_{LDPE}$)
Water (kg/kgLDPE)	2.45	$2.1 \cdot 10^{-6}$ \$/kg	$5.145 \cdot 10^{-6}$
Heat	602 kJ/kgLDPE	$9.95 \cdot 10^{-6}$\$/kJ	$4.74 \cdot 10^{-3}$
Electricity	724 kJ/kgLDPE	7.6 c/kWh	$1.53 \cdot 10^{-2}$
$FeCl_3$	0.021 kg/kgLDPE	0.7\$/kg	$1.55 \cdot 10^{-2}$
NaOH	0.0284 kg/kgLDPE	0.626\$/kg	$1.78 \cdot 10^{-2}$
Polyelectrolyte, assumed to be starch[a]	$2.68 \cdot 10^{-3}$ kg/kgLDPE	0.629\$/kg	$1.68 \cdot 10^{-3}$
TOTAL			**$5.50 \cdot 10^{-2}$**

[a]Starch is a polyelectrolyte use in water purification.[6]

The CAPEX is determined following the cost estimator tool of Peters[5] for most of the units. Only the washer[7] and thermal dryers[8] are estimated with the cost provided by industrial vendors and are scaled-up with a six-tenth rule.[9] The overall CAPEX as a function of the scale is computed as presented in Eq. (S-6).

$$CAPEX\left(\frac{\$}{s}\right) = 0.0039 \cdot f_{LDPE}\left(\frac{kg}{s}\right)^{0.65527} \qquad \text{(S-6)}$$

S-1.4 Mechanical recycling

Mechanical recycling only requires adding one extruder after the pretreatment of the plastic. The electricity and heat requirements of the extruder are computed following Larrain et al.,[2] obtaining the OPEX given in Eq. (S-7). The overall plant cost (pretreatment+extruder) is determined with the cost estimator of (2). The CAPEX is estimated as presented in Eq. (S-8).

$$OPEX\left(\frac{\$}{s}\right) = 4.8286 \cdot 10^{-3} \cdot f_{LDPE}\left(\frac{kg}{s}\right) \tag{S-7}$$

$$CAPEX\left(\frac{\$}{s}\right) = 0.0113 \cdot f_{LDPE}^{\ 0.8202} \tag{S-8}$$

S-1.5 Gasification

LDPE gasification can be carried out with several gasifying agents (e.g. air, steam). Following the review paper of Lopez et al.[10] one of the processes with highest yields is obtained by a fluidized bed with olivine as a heat transfer solid in the bed. The yields used for modeling the reactor are taken from Arena et al.[11] Two process alternatives are modeled with Aspen Plus as presented in Figure S-3 and Figure S-4. In the Aspen Plus simulation, PolyNRTL package is employed for the properties of the components. In this package we modify the LDPE heat capacities in solid and liquid form with reports in the literature,[12,13] and the formation enthalpy is taken from the National Bureau of Standards.[14] The first process (Figure S-3) focuses on the production of H_2 and syngas from LDPE, and it has 2 alternatives depending on the use of H_2. In the first process H_2 is separated by a PSA[15] obtaining a pure product and the remaining stream is used for producing power to be used as energy recovery in the system. In the second case, all the H_2 can be burnt into a turbine to produce power. The OPEX, product, and CAPEX are given in Table S-2.

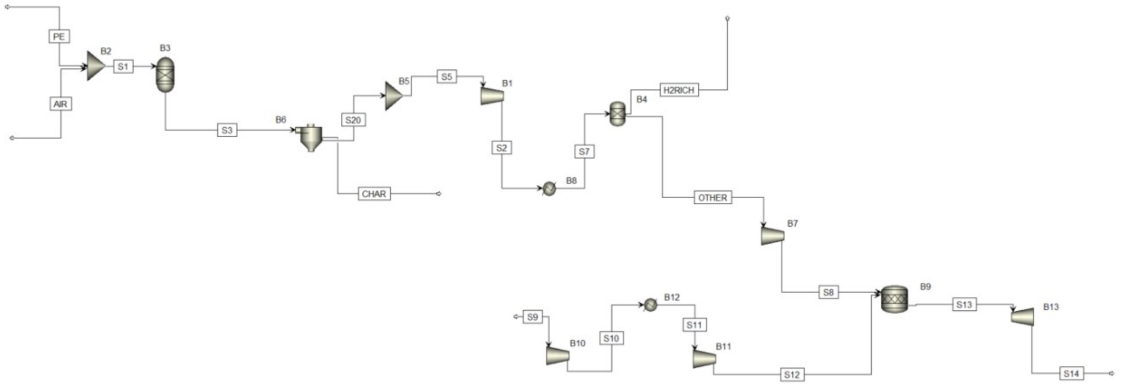

Figure S-3. Gasification to produce H_2 and power.

Another alternative process employs reforming[16] for transforming the hydrocarbons formed in the gasification to increase the yield to H_2 or syngas. The process is presented in Figure S-4.

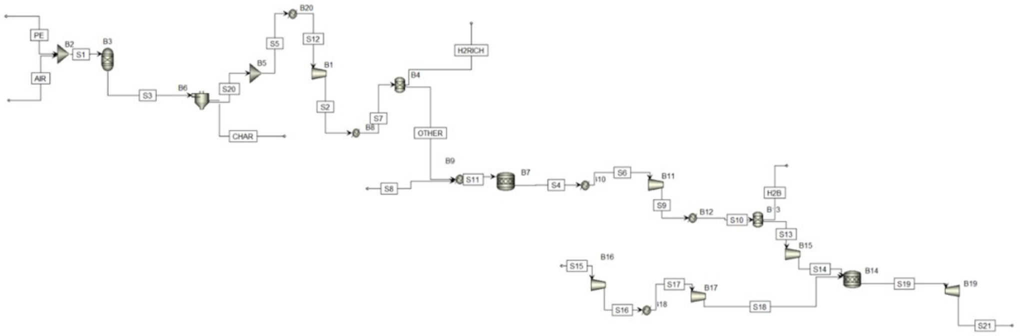

Figure S-4. Intensified process to produce H_2 followed by reforming and water gas shift.

Previous gasification uses consider only power, syngas, and hydrogen as finished products. However, the syngas produced can also be used to synthesize several components (e.g. methanol, ethanol, DME, fuels by Fischer-Tropsch).[17,18] The production of fuels is less competitive and more emission-intensive than other direct methods of production such as hydrothermal liquefaction. Thus, for comparison and selection of a finished product, the process is constrained to the production of methanol. Methanol production requires removing the N_2 and unreacted hydrocarbons produced in the reformer by means of a bed. Then, the syngas is sent to the synthesis and separation sections presented in Figure S-5. The methanol synthesis reactor is modeled at 200ºC and 50 bar using the conversions given in Hernández and Martín.[19]

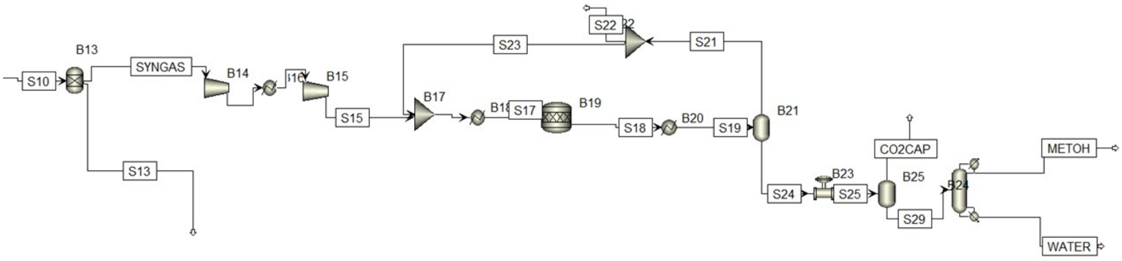

Figure S-5. Production of methanol from gasification and synthesis.

Table S-2. Comparison of process yields and CAPEX functions. In the CAPEX, y is the CAPEX in (\$/s), and F is the flowrate of the inlet in (kg/s).

Process	**OPEX (\$/kg$_{\text{LDPE}}$)**	**Product Yield (per kg of LDPE)**	**CAPEX (y=a*F^(b))**	
			a	**b**
Gasification to H_2	0.01581	0.089222 (kgH2)	0.177	0.9037
Gasification and Reforming of H_2	0.01131	0.091253 (kgH2)	0.2432	0.8887
Gasification to Power	-	2.721 (MW)	0.03325	0.9474
Gasification to MetOH	0.06385	1.1975 (kg of MetOH)	0.2538	0.8402

S-1.6 Hydrothermal liquefaction

Hydrothermal liquefaction is another high-temperature technology that produces a mixture of paraffins with an adequate octane ratio by reacting the LDPE with water at high temperatures. The reactor is modeled as a stochiometric reactor following the distribution given by Jin et al.[20] The product is first separated from the water in a decanter. Then, it is sent to a fractionation column where it is separated into diesel, gasoline, and LPG, see Figure S-6. The summary with the OPEX, production rates, and CAPEX is given in Table S-3.

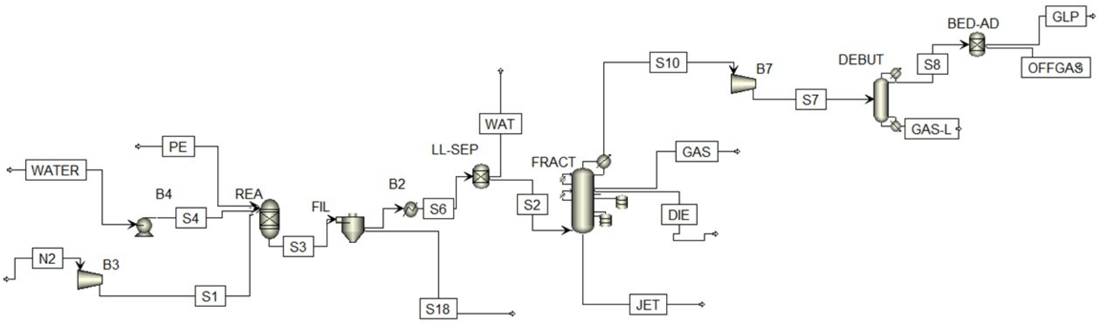

Figure S-6. Production of GLP, gasoline, diesel, and jet fuel from LDPE via HTL.

Table S-3. Summary of yields, OPEX, and CAPEX for HTL process.

Product type	Product Yield (Kg/kgLDPE)	OPEX	CAPEX	
			a	b
GLP	9.04E-02	0.192953	0.0417	0.564
Gasoline	3.23E-01			
Diesel	3.00E-01			
Jet fuel	2.25E-01			

S-1.7 Hydrocracking

Hydrocracking is modeled following the work of Liu et al.[21] The process operates at mild temperatures, 250ºC, and 1 atm, and it requires the use of H_2 for cracking the LDPE, and it has higher selectivity to produce paraffin carbons in the range of a gasoline fraction. Paraffins are separated into several fractions using distillation columns, as given in Figure S-7. H_2 is a valuable component that is recovered by a PSA membrane placed after the separation of the hydrocarbons. A summary of the operating costs, yields, and CAPEX is given in Table S-4.

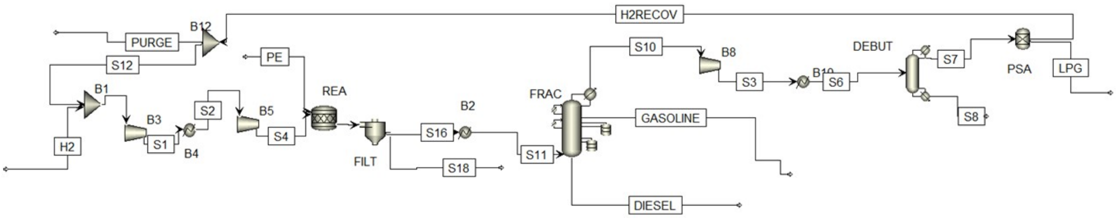

Figure S-7. Model for the hydrocracking process.

Table S-4. Summary of yields, OPEX, and CAPEX for the hydrocracking process.

Product type	Product Yield (Kg/kgLDPE)	OPEX	CAPEX	
			a	b
GLP	0.101375	0.100488	0.031	0.5818
Gasoline	0.722			
Diesel	0.039			

S-1.8 Hydrogenolysis

Hydrogenolysis is modeled by following the distribution of components and operating conditions reported in the work of Wang et al.[22] The technology works in mild conditions of temperature and pressure leading to a wide range of hydrocarbons (mixture of paraffins and olefins from C1 to C30), but with a higher selectivity to C30's, which can be used as lubricants. The separation of hydrocarbons is performed employing a fractionation column and a debutanizer. The hydrocarbons that are not recovered in the debutanizer are finally burnt to produce power. The process is given in Figure S-8. The operating costs, yields to the products, and CAPEX values are summarized in Table S-5.

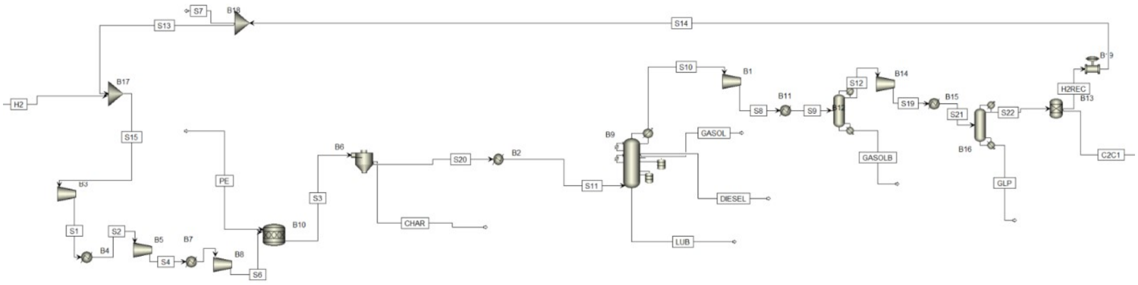

Figure S-8. Hydrogenolysis of LDPE.

Table S-5. Summary of yields, OPEX, and CAPEX for Hydrogenolysis process.

Product type	Product Yield (Kg/kgLDPE)	OPEX	CAPEX	
			a	b
Lubes	0.1903	0.047845	0.10026	0.5179
Diesel	0.2000			
Gasoline	0.1981			
GLP	0.0585			

S-1.9 Pyrolysis

Pyrolysis is modeled following our previous work.[23] Two types of reactors are considered, a fluidized bed reactor and a MW slurry pyrolysis reactor. The fluidized bed is described in Zhao et al.,[24] where the reactor operates at 550ºC. The MW slurry pyrolysis reactor has shown a high selectivity to olefins that can be transformed into a wide range of highly value-added products. The first part of the overall processing is the reactor and removal of the impurities. The pyrolysis takes place at 370 ºC and 1 atm with a conversion of 92%.[25] The unreacted product is removed by filtration. The product is then cooled down at 30ºC followed by the separations processes. See this part of the process in Figure S-9. The operating costs and material produced are summarized in Table S-6. Due to the importance of these products and the costs involved in producing them, a more detailed superstructure with several alternatives is studied as presented in the following section S-1.10.

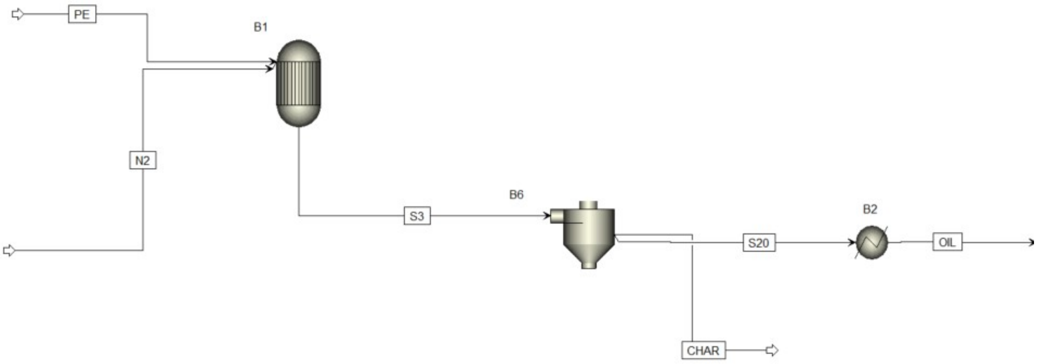

Figure S-9. Pyrolysis of LDPE.

Table S-6. Summary of consumptions and CAPEX for pyrolysis processes.

Type	**Consumption**	**CAPEX($/s)=a*F(kg/s)^(b)**	
		a	**b**
MW Reactor			
N2 (kg/kg LDPE)	0.007	0.1016	0.9917
Power (kJ/kg)	2723.20		
Ref (kJ/kg)	2688.38		
Fluidized bed reactor			
N2 (kg/kg LDPE)	0.7184	0.0305	0.449
Heat (kJ/kg)	3299.64		
Ref (kJ/kg)	1975.57		

S-1.10 Summary of the downstream products obtained by pyrolysis.

There is a wide range of products that can be generated from olefins. The first decision taken in the process is the selection of an oligomerization process to produce higher α-olefins or the separation of the olefins into the different fractions. α-olefins can be later used to produce lubricants in the production of linear alkyl benzene (LAB), a surfactant. On the other hand, a detailed separation for each of the components can lead to a multiple set of products. A summary of all the separation alternatives is given in Figure S-10 and Figure S-11.

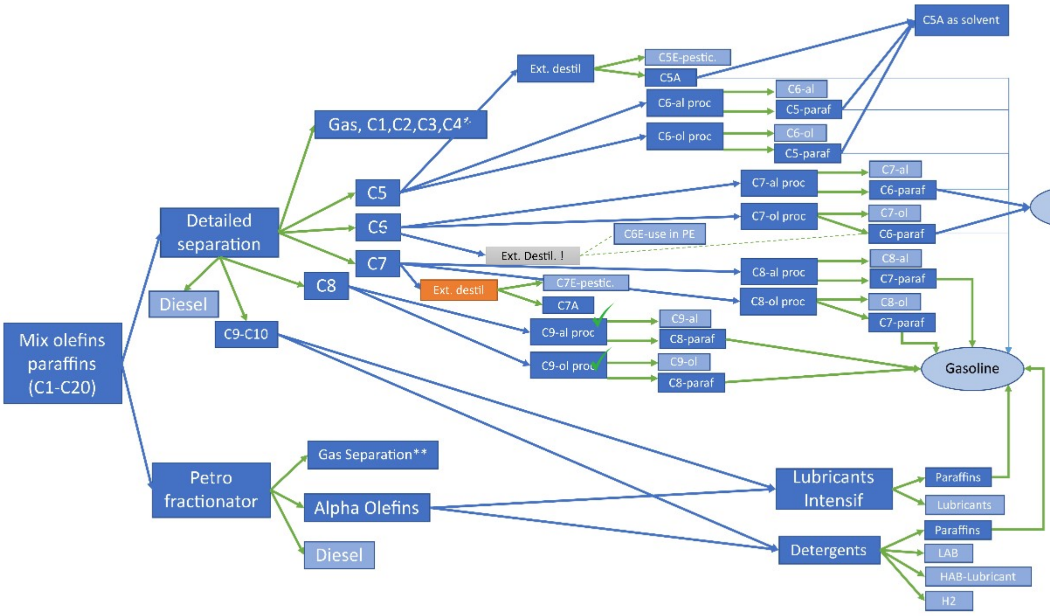

Figure S-10. Alternatives for the use of the naphtha from pyrolysis. Alternatives for the heavy fractions.

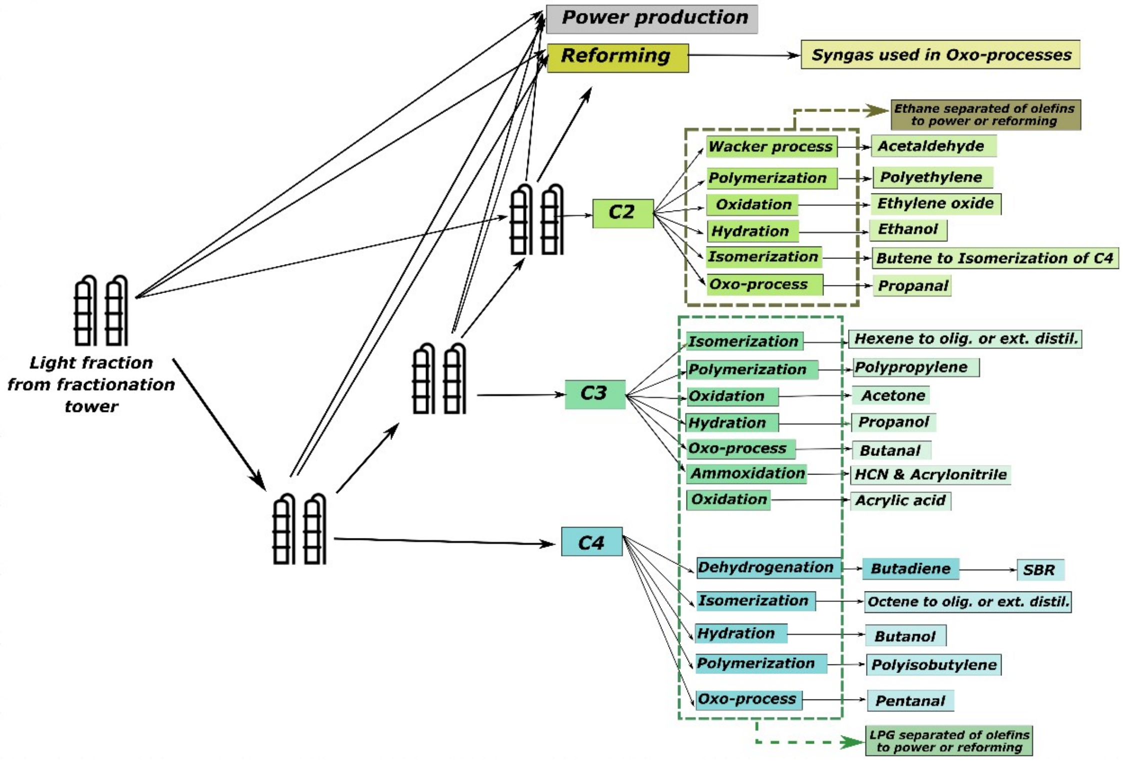

Figure S-11. Alternatives for the use of the separation and use of light fractions obtained from pyrolysis.

S-1.10.1 Integrated olefin oligomerization.

The first alternative studied is the oligomerization of the olefin mixture[26,27] obtained in pyrolysis to generate highly value-added products. The integrated process with energy recovery presented in our previous work[23] is considered as an alternative. See Figure S-12. A summary of the OPEX and CAPEX is given in Table S-7. The product obtained from the oligomerization can be sold as lubricant or used for the production of LAB, as given in the following subsection.

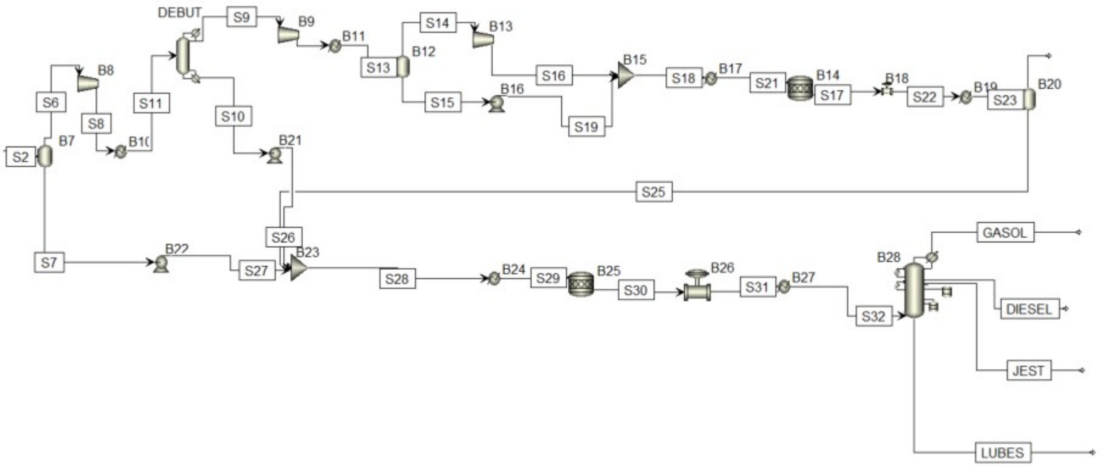

Figure S-12. Integrated process for the oligomerization of olefins to a-olefins.

Table S-7. Summary of consumptions and CAPEX for integrated oligomerization process.

Type	Consumption	CAPEX	
		a	b
Power (kJ/kg)	269.0269	0.075279	0.73325
Ref (kcal/kg)	2224.341		
Heat (kcal/kg)	1186.815		

S-1.10.2 Production of surfactants.

The product obtained from the oligomerization can be sold as a lubricant or used for the production of LAB. In the first alternative, the product can be sold as it is. In the second alternative, the LAB production process is based on the Detal process.[28–30] In the process modeling, there is no distinction of the type of alkylbenzene generated (HAB or LAB) leading to one distillation tower less than other processes presented. The ratio benzene: nonene (used as a representative compound from the olefins) is assumed to be 10.[30] The process is presented in Figure S-13. The summary of costs is given in table S-8.

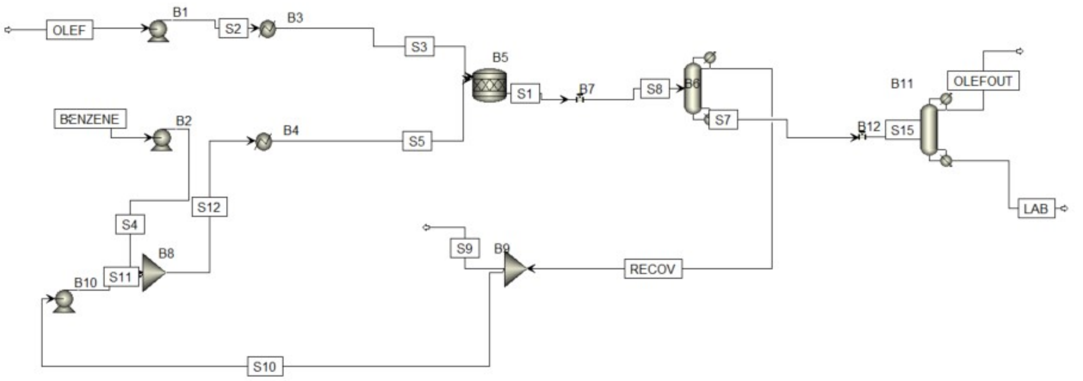

Figure S-13. Production of LAB from olefins and benzene.

Table S-8. Summary of consumptions and CAPEX for LAB process.

Type	Consumption	CAPEX	
		a	b
Power (kJ/kg)	3.38	0.0096	0.2806
Ref (kcal/kg)	159.042		
Heat (kcal/kg)	136.319		
Benzene	0.9		

S-1.10.3 Detailed separation.

An alternative to oligomerization is the detailed separation of the products generated. This detailed distillation divides the products in each of the carbon numbers. Then, each fraction is used to provide the most profitable components. The separation is performed by means of a tray of distillation columns as shown in Figure S-14. First, a fractionator is placed for separating a heavy fraction (Cn>8) that is sent to oligomerization, an intermediate liquid fraction, and a gas fraction. The liquid fraction is separated into each of the fractions by individual columns, and the gas fraction is considered to have several alternatives, as defined previously in Figure S-11. Each of the gas fractions can be separated into each of the carbons or they can also be sent to a turbine to generate power or to a reformer for generating H_2. A summary of the operating costs and CAPEX is given in Table S-9 for each of the columns involved in the separation.

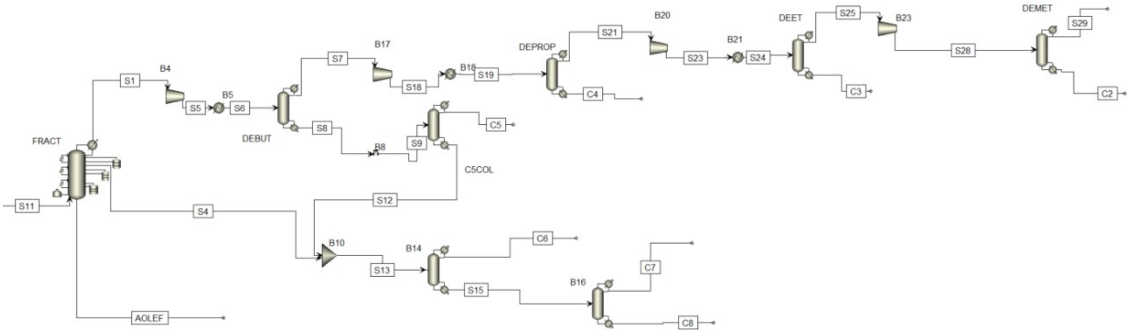

Figure S-14. Detailed separation. In the process, gas fractions are also assumed to be separated independently, but they can be separated one by one.

Table S-9. Summary of consumptions and CAPEX of fractionation columns. Refrigeration and heat are in kcal/kg$_{Feed}$ and Power is in kJ/kg$_{Feed}$.

Term	Value	kJ and kcal/kg feed	CAPEX (a)	CAPEX (b)
DESTIL 1			0.0096	0.7849
REF	-1414971	-1255.2724		
HEAT	1472200	1306.04239		
Fin	4058	1		
DEBUT			0.0103	0.3978
POWER	9.50E+04	35.13		
COOLING	328373	437.182988		
Fin	2704	1.00E+00		
DEPROP			0.0097	0.1289

POWER	4.60E+04	29.32		
cooling	247382	659.843002		
Fin	1569	1.00E+00		
DE-ETHANIZER			0.0089	0.1135
POWER	1.80E+04	17.95		
COOLING	193950	809.252991		
Fin	1003	1.00E+00		
DE METHANAIZER			0.0073	0.0942
POWER	4.00E+03	5.78		
COOLING	5074	30.6859682		
Fin	692	1.00E+00		
tower c5 from debut			0.0037	0.3798
HEATING	64981	206.107137		
COOLIGN	101740	322.699559		
Fin	1135	1.00E+00		
tower c6 from debut			0.0035	0.1977
HEATING	115907	302.14714		
COOLIGN	109948	286.613179		
Fin	1381	1.00E+00		
tower c7 - c8			0.0035	0.1376
HEATING	67915	334.008197		
COOLIGN	65209	320.7		
Fin	732	1.00E+00		

S-1.10.4 Use of C2 fraction

C2 fraction is composed of ethylene and traces of ethane. Ethylene is one of the most versatile chemicals used as a starting point in manufacturing more complex compounds (polyethylene, ethylene oxide used to produce ethylene glycol, chlorine compounds, ethanol, etc.). A summary of applications is given in Figure S-15.[31] However, not all the compounds presented in Figure S-16 have the same value and their production may involve other valuable materials. For example, vinyl-chloride requires using Cl_2[32] which is more valuable than ethylene and styrene requires benzene. Thus, the price and emissions of these chemicals are governed by those more valuable raw materials, and they are discarded in the formulation of the superstructure optimization.

Similarly, the polymers produced from those chemicals: polyvinyl chloride (PVC) and PET have only slightly higher prices than Polyethylene (PE). Thus, PE production is selected as a representative for simplification since it is a direct process and does not require other pricy compounds (e.g. Cl_2 in PVC production). Other alternatives to finished products are: the production of acetaldehyde, which can be later used in the production of perfumes, drugs, etc.;[33] ethylene oxide, a platform for other chemicals; propionaldehyde, another high valuable compound used in synthetic flavoring, disinfectant or preservatives;[34] ethanol by hydration and butene by oligomerization. In the following lines, the processes modeled for each alternative are presented.

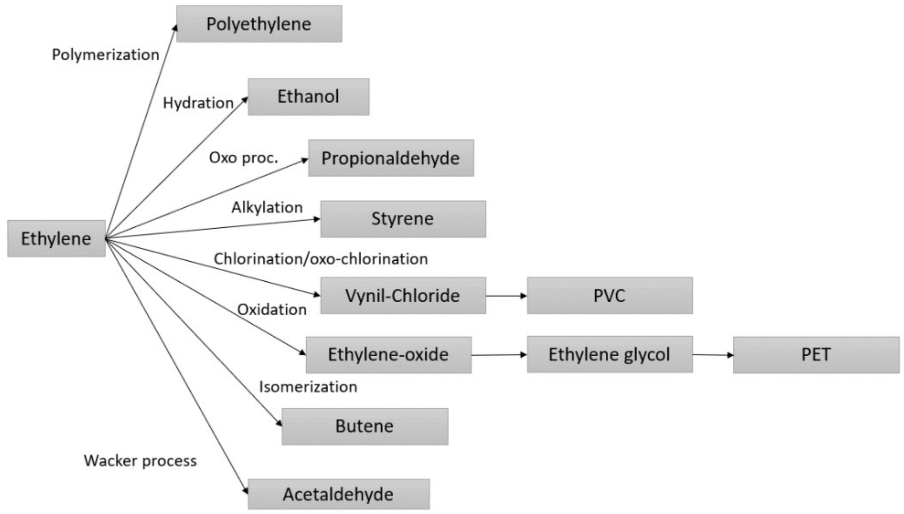

Figure S-15. Alternatives for the use of ethylene.

<u>The Wacker process for the production of acetaldehyde</u> from ethylene is modeled as presented in Figure S-16. The process first purifies the C2 stream to increase the concentration of ethylene. Then, it requires a catalytic oxidation reactor operating at 130ºC and 4 bar with $PdCl_2$ as a catalyst.[35] The acetaldehyde produced is finally recovered from the ethylene mixture with an extractive distillation. Water is employed to recover acetaldehyde and then a fractionation column is placed. A summary of the consumptions of the process and the surrogate model for the Capex is presented in Table S-10.

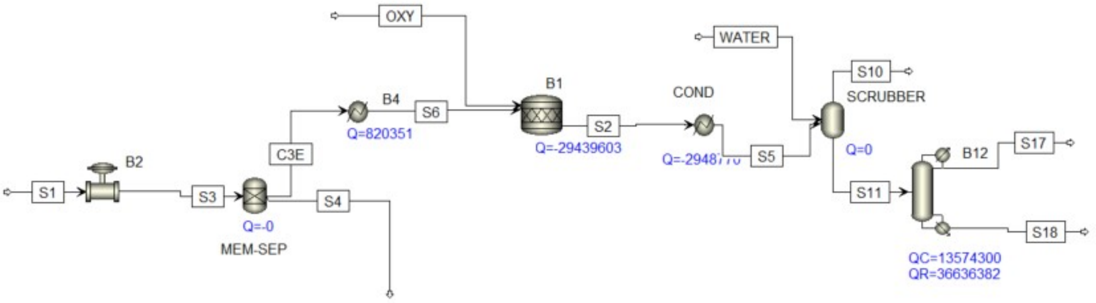

Figure S-16. Production of acetaldehyde from ethylene via Wacker Process, A) as defined in literature and B) represented in the model.

Table S-10. Summary of consumptions and CAPEX for Wacker process.

Type	Consumption (Kg or kcal/kgLDPE)	CAPEX	
		a	b
Ref	920.41	0.0086	0.7629
Heat	204.00		
Oxygen	0.278		
Purified Water	0.083		

<u>One alternative is the production of propanal by hydroformylation</u>. The oxo-process is modeled as presented in Figure S-17. In the process, hydroformylation occurs in a reactor operating at 16.5 bar and 175 ºC with $Co_2(CO)_8$ as catalysts.[36] A syngas to ethylene ratio of 1:1 is required. The yield achieved in the reactor is assumed to be 80%, based on the report for that type of catalyst for all the aldehydes.[37]To increase the yield, the unreacted products are recycled in a flash separator. The models for the consumptions and CAPEX are reduced with the parameters presented in Table S-11.

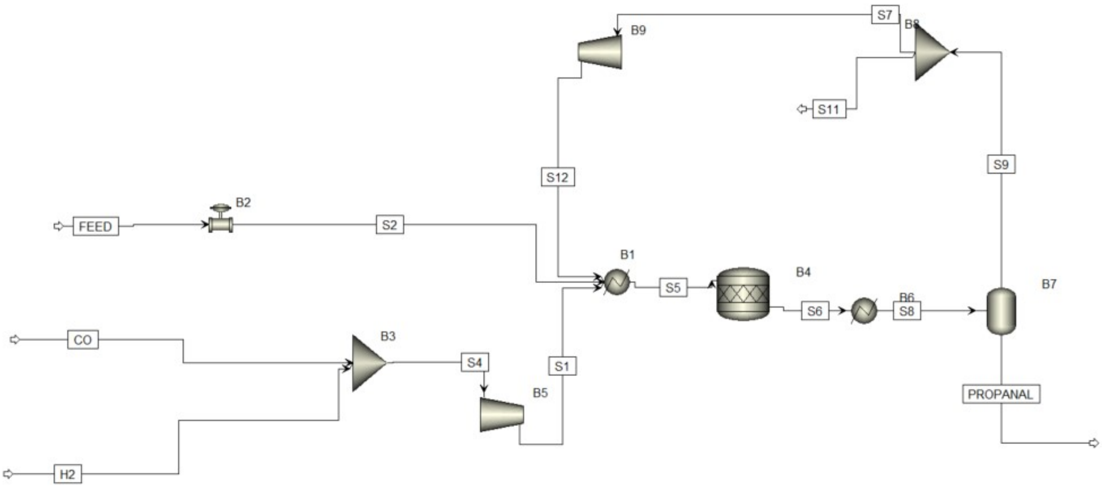

Figure S-17. Oxo process for the production of propanal from ethylene.

Table S-11. Summary of consumptions and CAPEX for Propanal production process.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	730.630833	0.0333	0.787
Heat (kcal/kg)	414.430278		
Power (kJ/kg)	2301		
CO (kg/kg)	0.694		
H2 (kg/kg)	0.083		

Polyethylene production is modeled following the Union Carbide process described in the patent US 4,543,399.[38,39] A fluidized bed reactor operating at T=54ºC and P=270psi is used in the process. The process flowsheet is presented in Figure S-18, and all the consumptions and costs are estimated using Aspen Plus. The PE obtained in the process if finally sent to an extruder, which is modeled as the one used for the mechanical recycling and also using Peter's Timmerhaus cost estimator for the CAPEX. A summary of the consumptions and surrogate model for the CAPEX is given in Table S-12.

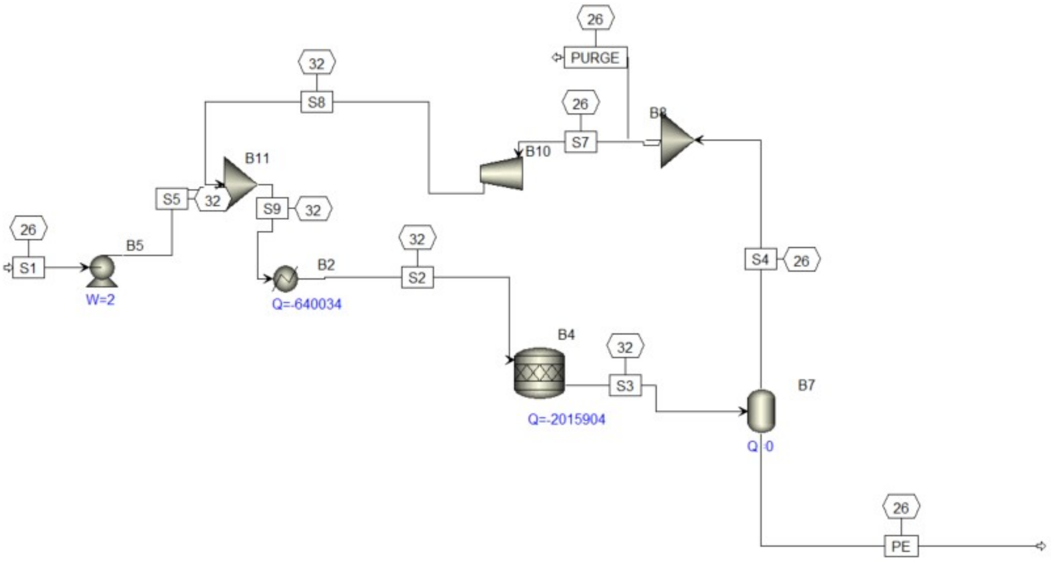

Figure S-18. Production of LDPE from ethylene.

Table S-12. Summary of consumptions and CAPEX for Polyethylene production process.

Type	Consumption	CAPEX	
		a	**b**
Ref (kcal/kg)	4327.49	0.0387	0.626
Heat (kcal/kg)	0		
Power (kJ/kg)	2707.2		

Ethylene to ethanol by hydration. Although it has been demonstrated not to be the most profitable route for ethanol production,[40] the process only requires water as raw material. In fact, the route followed is typically the opposite, using ethanol to produce ethylene since it is more profitable. Instead of these cons, the process has been modeled as addressed in Figure S-19. The hydration reactor requires steam with a steam: ethylene ratio of 2.4:1 at 60 bar and 246 ºC.[40] The conversion to ethanol is limited to 5% per pass. So ethylene needs to be recycled.[41] A summary of the consumptions and parameters for CAPEX estimation are given in Table S-13.

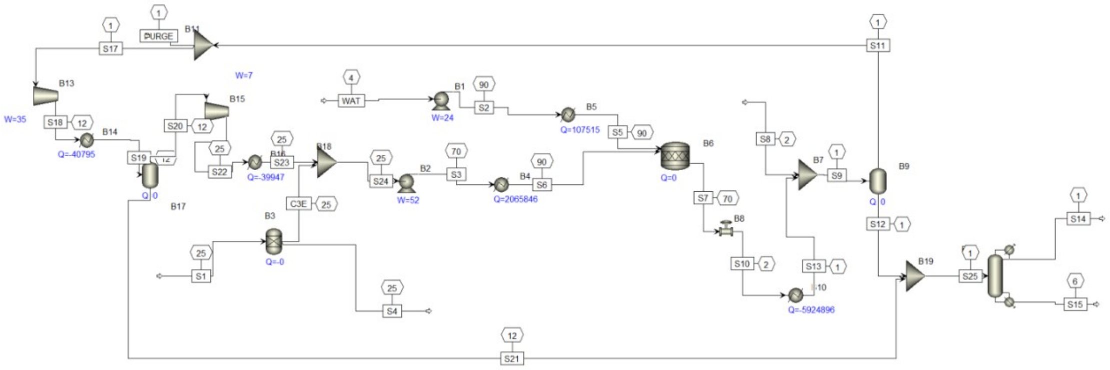

Figure S-19. Production of ethanol from ethylene.

Table S-13. Summary of consumptions and CAPEX for the ethanol production process.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	563.75	0.0507	0.41
Heat (kcal/kg)	270.61		
Power (kJ/kg)	7011		
Purified wáter (kg/kg)	0.801		

Ethylene oxide is one of the most widely used compounds obtained from ethylene. The production of ethylene oxide is carried out between 200 ºC and 300 ºC and pressures between 10 and 20 bar, with yields around 85%. The process flowsheet is modeled following the previous works[39] and presented in Figure S-20. The summary of the models for the consumptions and CAPEX is presented in Table S-14.

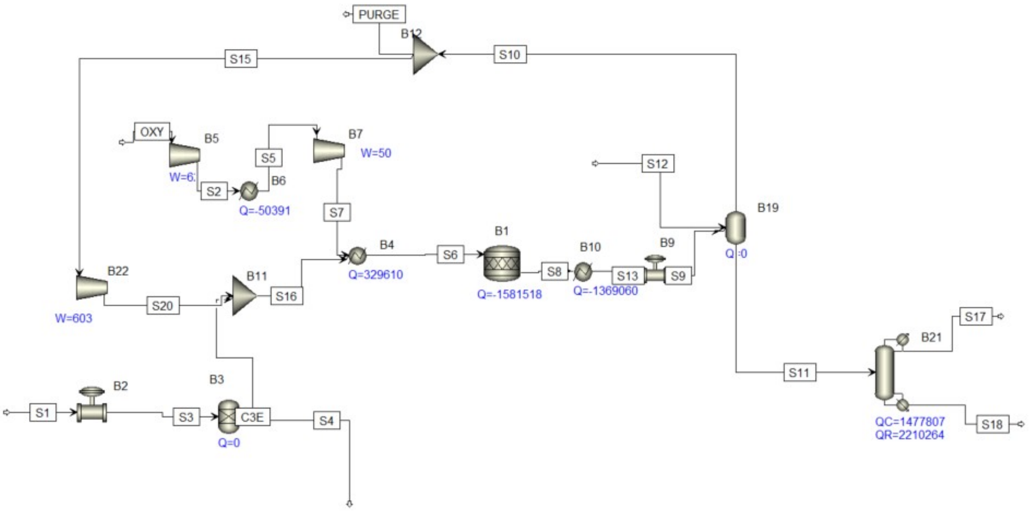

Figure S-20. Process flowsheet to produce ethylene oxide from ethylene.

Table S-14. Summary of consumptions and CAPEX for ethylene oxide production process.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	1048.83	0.0351	0.3707
Heat (kcal/kg)	4.6984		
Power (kJ/kg)	56.7		
Purified wáter (kg/kg)	0.025		
Oxygen	0.25		

Isomerization to butene is modeled following the patent[26] as done for the light olefins fraction in the integrated oligomerization process presented before. In this process, the reactor converts 90% of the ethylene at 70 bar and 200 ºC with ZSM-5 zeolites as a catalyst.[26] Once oligomerization occurs in the fixed bed reactor, the higher olefins obtained as a product are separated in a flash vessel from the paraffins. A summary of the consumptions and parameters for the estimation of the CAPEX with a surrogate is given in Table S-15.

Table S-15. Summary of consumptions and CAPEX for isomerization of ethylene.

Type	Consumption	CAPEX	
		a	**b**
Ref (kcal/kg)	292.78	0.0146	0.3881
Heat (kcal/kg)	5.37		
Power (kJ/kg)	123.50		

S-1.10.5 Use of C3 fraction

Olefin C3 fraction can also be used to produce a wide variety of chemicals summarized in Figure S-21.[42] In a similar way that for ethylene, some components can be removed from scratch since olefin production is not the main contributor to the costs. The other additional raw materials needed require other processes with no simple routes from plastic waste. For example, the main cost of cumene is given by the benzene used as raw material, which is produced by the catalytic hydration of a hydrocarbon mixture, and the current plastic waste route requires a similar process.

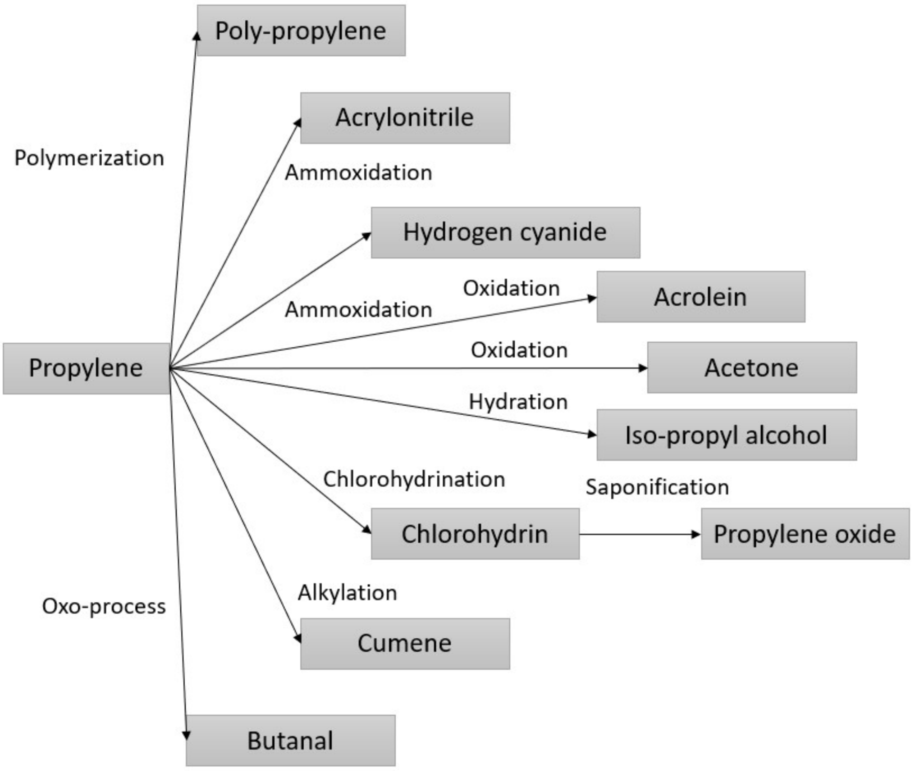

Figure S-21. Summary of propylene uses.

Polypropylene production Polypropylene is generated following the same Union Carbide process described previously for LDPE production and the patent 4,543,399.[38] The operating temperature of the fluidized bed is reduced to 60ºC at a pressure of 270 psig. The results obtained for the fluxes and CAPEX are summarized in Table S-16.

Table S-16. Summary of fluxes and CAPEX for the polypropylene-Union Carbide production process.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	466.3553	0.0143	0.3561
Heat (kcal/kg)	0		
Power (kJ/kg)	1076.349		

Butanal production by hydroformylation. We follow the low-pressure, 1.8 MPa, oxo process developed by Union Carbide.[43] This process employs Rhodium as a catalyst in high boiling thick oil at 97 ºC.[44] The reaction mixture is separate from volatile components in a falling film evaporator. The process is presented in Figure S-22. A summary of the consumptions and correlation generated for estimating the CAPEX is given in Table S-17.

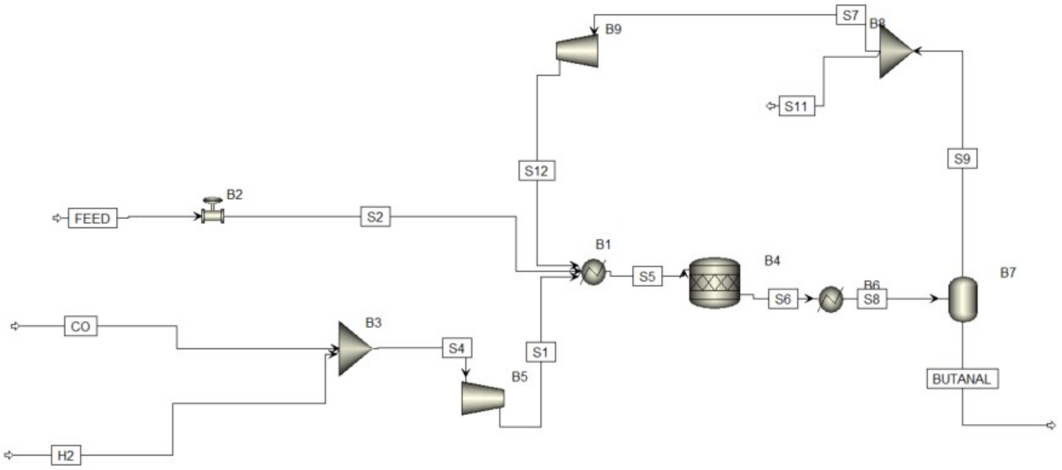

Figure S-22. Butanal production from propylene.

Table S-17. Summary of fluxes and CAPEX for the butanal production process.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	140.763	0.0308	0.5197
Heat (kcal/kg)	22.2096		
Power (kJ/kg)	0.29945		
H2 (kg/kg)	0.6404057		
CO (kg/kg)	0.6730794		

Oxidation of propylene to acetone

The process for producing acetone from propylene is carried out following the Wacker process as previously designed for acetaldehyde production.[45] The oxidation occurs at 110 ºC and 10 atm, achieving high conversion rates, ~94%.[46] The process is presented in Figure S-23 and a summary of the consumptions and function for estimating the Capex is given in Table S-18.

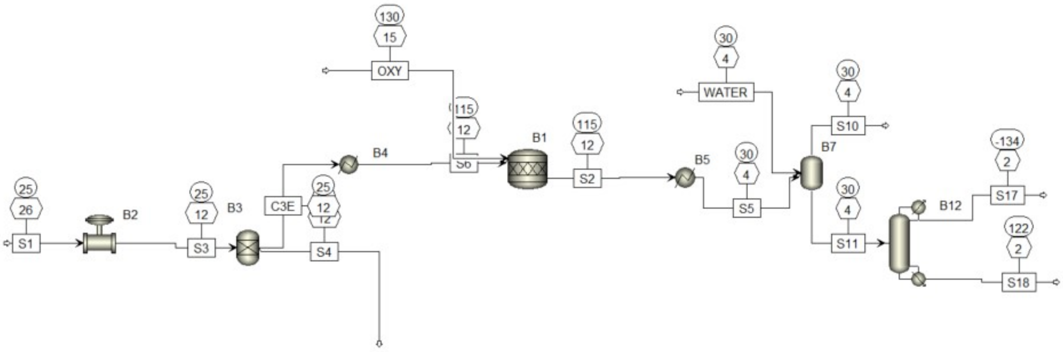

Figure S-23. Oxidation of propylene to acetone.

Table S-18. Summary of fluxes and CAPEX for the production of acetone from propylene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	1378.611	0.0099	0.7161
Heat (kcal/kg)	202.3686		
Power (kJ/kg)	-		
Water (kg/kg)	0.0556		
O_2 (kg/kg)	0.2500		

<u>Hydration for the production of propanol.</u> Production of iso-propanol by hydration of propylene is carried out following direct hydration like in the Texaco process.[47,48] In the process, hydration takes place in a strong acid ion exchange membrane at high pressure, 80-100 atm, and low temperature, 150 ºC.[49] The process is presented in Figure S-24, and the summary of consumptions and CAPEX is given in Table S-19.

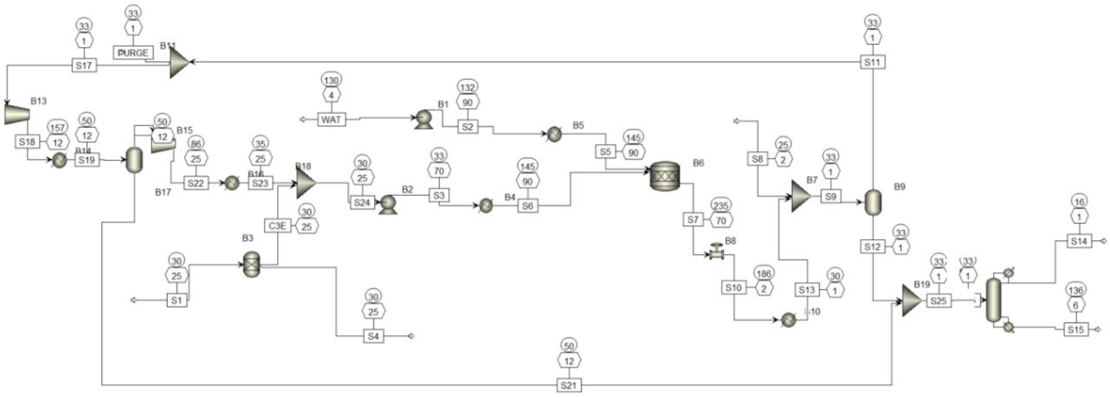

Figure S-24. Production of propanol via direct hydration.

Table S-19. Summary of fluxes and CAPEX for the production of propanol from propylene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	229.778	0.0393	0.6846
Heat (kcal/kg)	324.722		
Power (kJ/kg)	14.9		
Water (kg/kg)	0.2		

Ammoxidation to HCN and acrylonitrile

One alternative use is the production of acrylonitrile, a valuable monomer employed as pesticide and in the production of plastics, rubbers. The production of acrylonitrile simultaneously generates HCN through the Sohi process. The process is presented in Figure S-25, and it requires a Propylene:NH_3:Air ratio of 1:1.1:8.1, achieving a conversion of ~80%.[50,51] Once Propylene reacts, the product is sent to a set Quench neutralizer where the unconverted ammonia reacts with a sulfuric acid diluted solution to be transformed into an ammonium sulfate. After removing the ammonia, the light gases (unreacted air) are separated in a stripping column. Then, the organic gases are sent to a set of fractionation columns; where HCN is recovered first, and acrylonitrile is separated.[52] A summary of the consumptions in the process and correlation for CAPEX estimation are given in Table S-20.

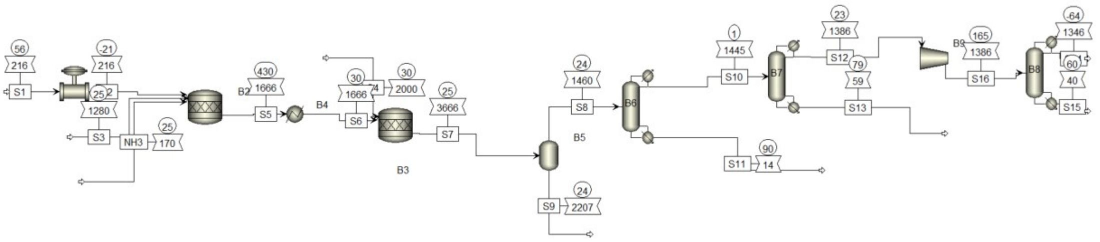

Figure S-25. Production of acrylonitrile from propylene.

Table S-20. Summary of consumptions and parameters for the CAPEX correlation for acrylonitrile production from propylene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	52.14	0.0769	0.2664
Heat (kcal/kg)	1191.34		
Power (kJ/kg)	0.342		
Water (kg/kg)	6.190		
NH3 (kg/kg)	0.882		

Acrylic acid production via oxidation of propylene

The production of acrylic acid is performed by means of partial oxidation with oxygen and steam following the Lurgi process.[53] A description of the process in given in Figure S-26. Acrylic acid is produced through a chain reaction: In the first reaction, propylene is oxidized to acrolein, and in the second reaction, acrolein forms acrylic acid.[52] A side reaction also results in acetic acid (~7%). The products obtained at the outlet are sent to an extractive distillation system. First, an extraction tower where they are extracted with methyl-isobutil ketone, and then a distillation tower to separate the acids.[53] The off-gas obtained in extraction is mainly composed of the unreacted propylene recycled back to the reactor.

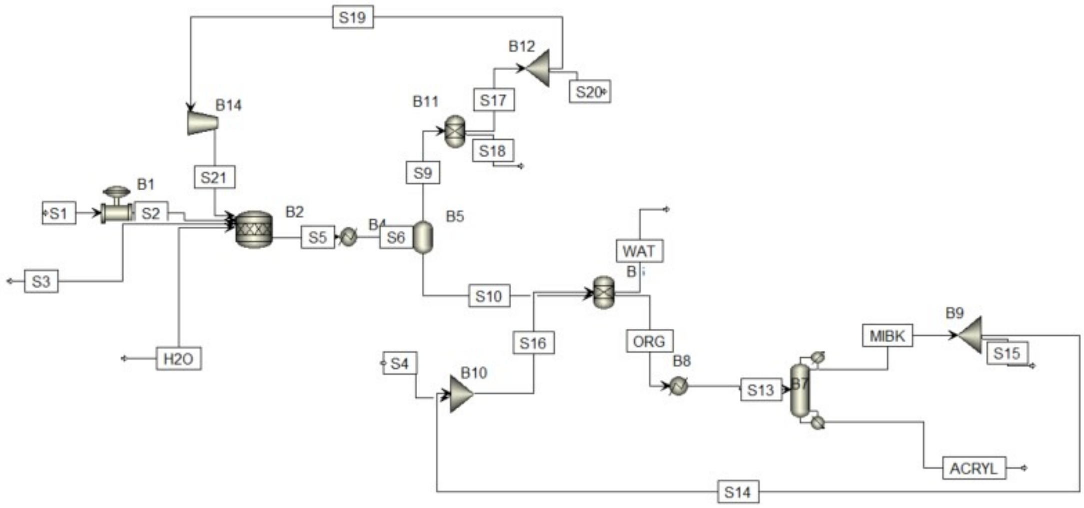

Figure S-26. Production of acrylic acid from propylene.

Table S-21. Summary of consumptions and parameters for the CAPEX correlation for acrylic acid production from propylene.

Type	Consumption	CAPEX	
		a	**b**
Ref (kcal/kg)	2592.0522	0.0874	0.537
Heat (kcal/kg)	425.5383		
Power (kJ/kg)	0.037354		
Water (kg/kg)	2.3346		

S-1.10.6 Use of C4 fraction

The C4 fraction of olefins has multiple alternatives that are summarized in Figure S-27. The two main isomers obtained by thermodynamic equilibrium in pyrolysis are iso-butene (≈70%) and 1-butene (≈25%). Isobutene can be used to produce multiple products such as polymers, fuels (MTBE, ETBE), solvents, or oxidants. All the possible products presented in Figure S-27 are studied except MTBE since the interesting route is the opposite (iso-butene has nearly the double value of MTBE) so it will never be a realistic or interesting alternative, even from an environmental point of view. The remaining options for i-butene are studied such as the production of polyisobutylene, the isomerization to alpha olefins assumed to be iso-octone, the hydration to tert-butanol, and the hydroformylation to pentanal. Furthermore, one alternative for n-butene is also considered: butadiene production by dehydrogenation and its later use as styrene-butadiene-rubber (SBR). Other polymers such as neoprene and acrylonitrile-butadiene-styrene (ABS) can also be produced from butadiene, but the analysis is simplified, including only SBR production since in the remaining products, the changes would be given by the additional components (Styrene, acrylic acid) instead of butadiene production.

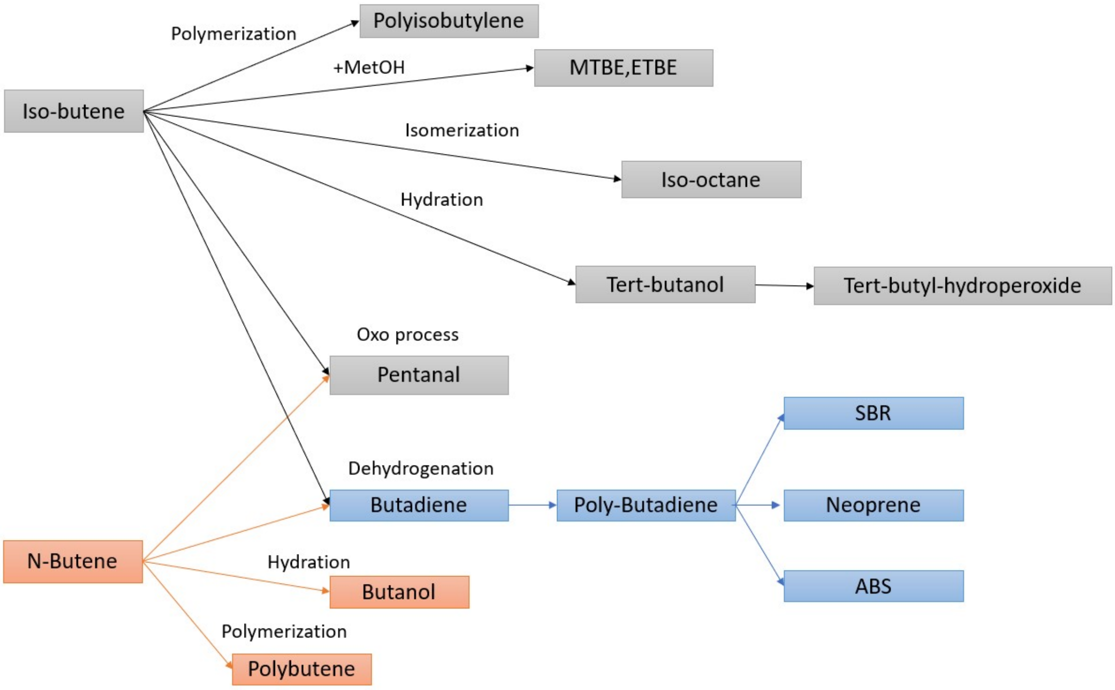

Figure S-27. Uses of butene compounds.

<u>Polyisobutylene and polybutylene</u> are modeled following the Exxon process based on the polymerization at a low temperature, -40ºC, in a hexane solution.[54] The process is modeled as presented in Figure S-28. A summary of the fluxes and the function parameters for estimating the CAPEX is given in Table S-22.

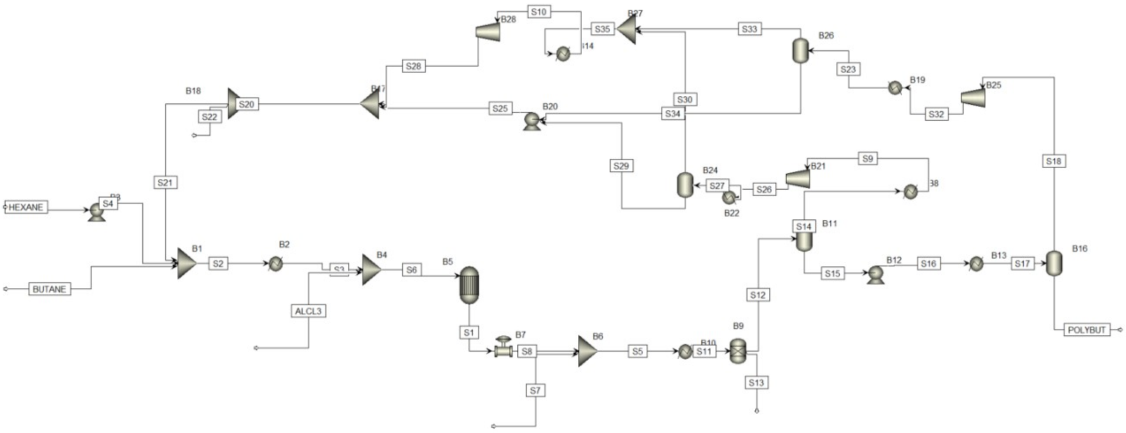

Figure S-28. Production of polybutylene from butene.

Table S-22. Summary of consumptions and function for CAPEX estimation for the production of polybutylene from butene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	138.7542	0.0485	0.3252
Heat (kcal/kg)	61.15373		
Power (kJ/kg)	810.801		
Power refrig (kJ/kg)	264.8403		
Water (kg/kg)	1.442687		

Hexane (kg/kg)	0.416346		
$AlCl_3$ (kg/kg)	0.009682		

Oligomerization of butene to larger chains takes place on acid catalysts like zeolites at temperatures around 100 ºC, and pressures ~1.7 MPa.[55] The process is similar to the previously described but operates at lower pressures. It achieves a high conversion, ~90%, being the alpha olefins separated from paraffins in a flash separator. The process is presented in Figure S-29, and a summary of the consumptions and capex is given in Table S-23.

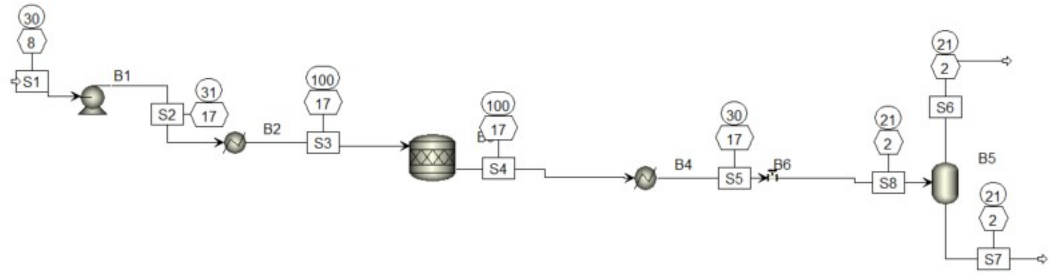

Figure S-29. Isomerization of butene to alpha olefins.

Table S-23. Summary of consumptions and function for CAPEX estimation for the isomerization of butene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	110.65	0.0047	0.2644
Heat (kcal/kg)	6.48		
Power (kJ/kg)	1.60		

Hydration of butene to butanol. Hydration of butene for butanol production is modeled following the Saudi Aramco process that requires the hydration of a mixture of butenes at high pressures, 68 bar, and 150ºC, with conversions ~14% using ZSM-5 activated zeolites as catalysts. The process is the same as the one followed for propanol production. Only the conversion is low, only 14% is converted to butanol per pass.[56] Furthermore, the conversion is not selective to a single C4 alcohol, and it produces a mixture of alcohols that can be used as additives for fuels. The process is depicted in Figure S-30. A summary of the consumptions and CAPEX function is given in Table S-24.

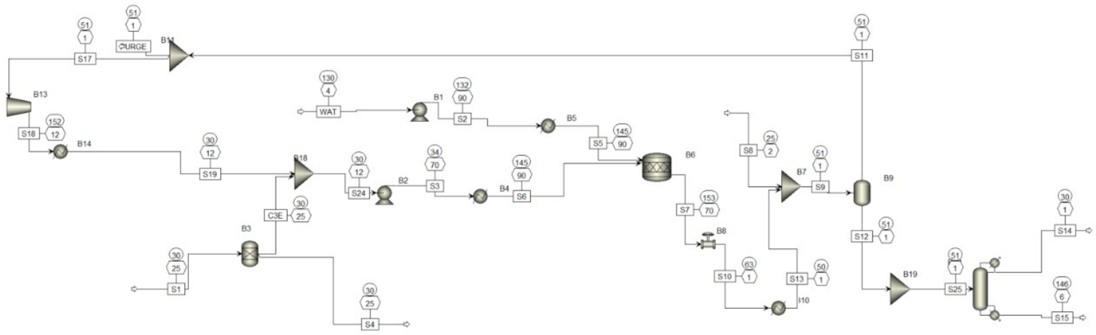

Figure S-30. Hydration of butene to butanol.

Table S-24. Summary of consumptions and function for CAPEX estimation for the hydration of butene to butanol.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	1483.64	0.0295	0.2438
Heat (kcal/kg)	1085.33		
Power (kJ/kg)	736.62		
Water (kg/kg)	0.808		

<u>Dehydrogenation of butylene to butadiene</u> is one interesting route since this monomer is employed in producing polymers like styrene-butadiene rubber (SBR). The dehydrogenation process is modeled following the Houndry Catadiene process.[56The]The C4 stream is sent to a catalytic reactor operating at 650ºC and 2 atm under chromium oxide as a catalyst, obtaining a conversion ~20% per pass. Butadiene is later separated (concentration achieved of 50%) with extractive distillation using acetone as extractant.[57]. The process is summarized in Figure S-31.

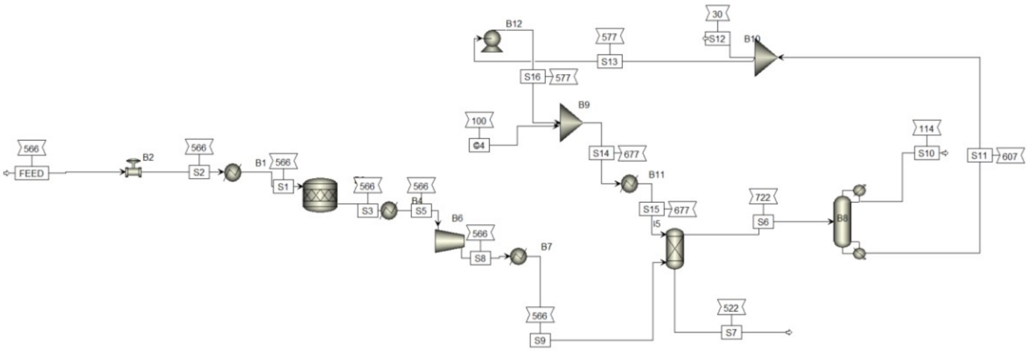

Figure S-31. Dehydrogenation process for the production of butadiene from butene and butane.

Once butadiene is selectively separated, it is polymerized with styrene in stirred tank reactors at 0.5 MPa and 25ºC.[58,59] After polymerization, SBR is separated by a vacuum separator to recover the gases, followed by a neutralization column that recovers the water employed in the polymerization, see the process in Figure S-32. The summary of the consumptions of both processes and the CAPEX are given in Table S-25.

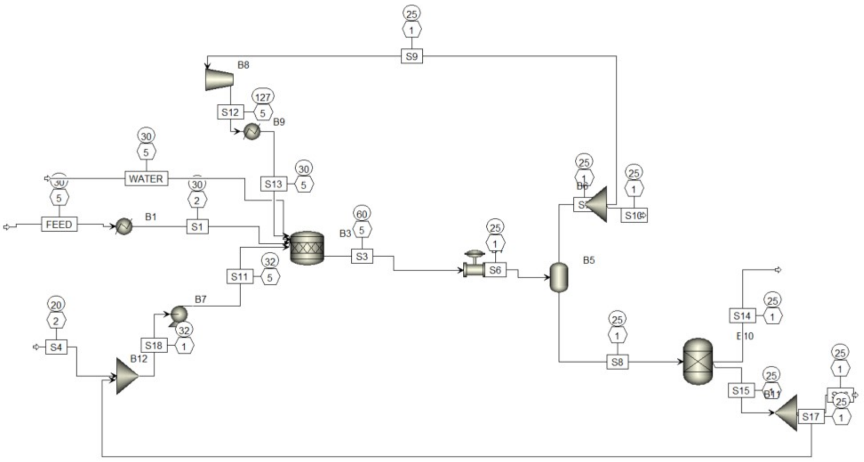

Figure S-32. Production of SBR from butadiene and styrene.

Table S-25. Summary of consumptions and function for CAPEX estimation for the production of SBR.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	329.72	0.0657	0.5157
Heat (kcal/kg)	0		
Power (kJ/kg)	2571		
Water (kg/kg)	0.167		
Styrene (kg/kg)	0.35		

Oxo-process for pentanal production. The last alternative for the C4 fraction considers the production of pentanal by hydroformylation of butene following the ExxonMobil patent.[60] The oxo-process is similar to those presented previously, where syngas rea with butenes in a hydroformylation reactor. However, the operating conditions of the hydroformylation reactor require operating at 15 bar, and ~95 ºC, with an H_2 to CO molar ratio of 5:1. The conversion per pass is around 60% so that the unreacted components are recycled, as given in Figure S-33. The summary of the consumptions and CAPEX model are shown in Table S-26.

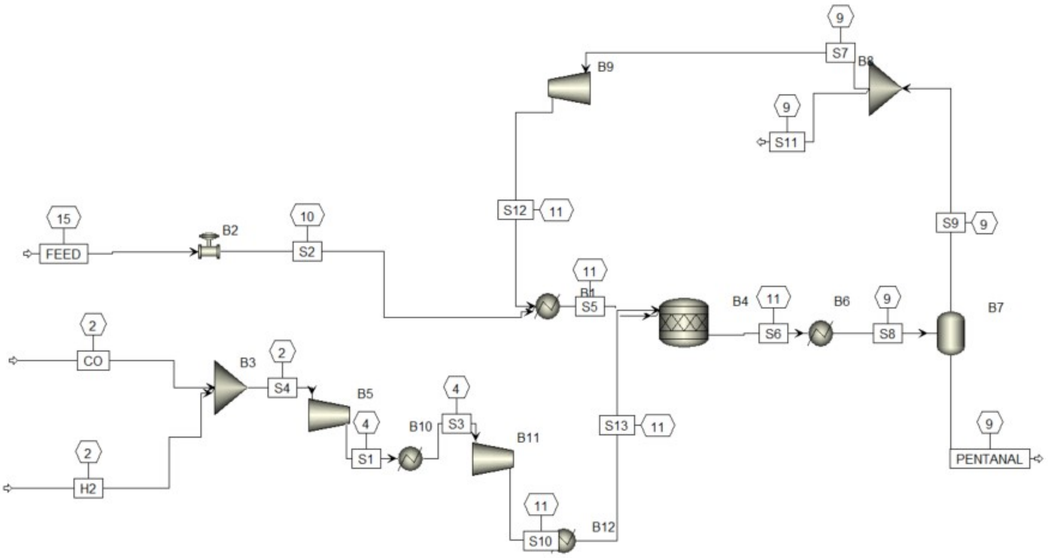

Figure S-33. Production of pentanal from butylene.

Table S-26. Summary of consumptions and function for CAPEX estimation for the production of pentanal.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	768.71	0.0273	0.3169
Heat (kcal/kg)	0.0		
Power (kJ/kg)	101.6809		
CO (kg/kg)	0.17384		
H_2 (kg/kg)	0.012809		

S-1.10.7 Use of C5 fraction

Olefins produced in the C5 fraction can be separated independently to produce pentane and pentene, which can be used as solvents or plasticizers without any other modification, or they can be transformed into hexanal, an aldehyde with smell to grass widely used in the perfume industry.

Hexanal production The production of hexanal is carried out through the oxo process operating at 45 bar and 110 ºC, with yields of ~90%.[61,62] The process is similar to the one presented for the production of other aldehydes. Only the operating conditions are different. A summary of the consumptions of syngas, utilities, and the function employed for estimating the CAPEX is given in Table S-27.

Table S-27. Summary of consumptions and function for CAPEX estimation for the production of hexanal.

Type	Consumption	CAPEX	
		a	b

Ref (kcal/kg)	158.84249	0.0457	0.1086
Heat (kcal/kg)	0		
Power (kJ/kg)	278.9268		
CO (kg/kg)	0.083277		
H2 (kg/kg)	0.005948		

Separation of pentene

As an alternative to hydroformylation, one option for processing pentene is to extract it from the mixture with paraffins and sell it as a solvent. The process for separating pentene from pentane is performed by extractive distillation employing acetone as solvent.[63,64] After extraction, and the separation of pentene from acetone by distillation, acetone is recycled to minimize operating costs. A summary of the consumptions and CAPEX is given in Table S-28.

Table S-28. Summary of consumptions and function for CAPEX estimation for the production of pentene.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	57.0474502	0.0316	0.5294
Heat (kcal/kg)	66.3914218		
Power (kJ/kg)	0		
Acetone (kg/kg)	0.150455		

S-1.10.8 Use of C6 to C8 fractions

Similarly to C5 fraction, C6 to C8 fractions are very valuable products since they are used in specialized industries like flavors, perfumes, plasticizers, or pesticides. The two alternatives considered for each of these fractions are the separation of the olefins and paraffins by means of extractive distillation for them to be used independently and the oxo-process for producing aldehydes and alcohol-based components. Since the processing of aldehydes requires less processing (alcohols are obtained by reacting aldehydes with hydrogen),[65] the process is assumed to stop as aldehydes from the oxo process. Apart from aldehydes, the other alternatives considered for these fractions are the separation of the olefins for being sold as solvents and the oligomerization to larger chains to produce lubes and detergents. Extractive distillation is assumed to be carried out similarly and with the same consumptions as for separating pentene from pentane. The production of aldehydes and the oligomerization are summarized in the following paragraphs.

Aldehydes production by hydroformylation. Heptanal, octanal, and nonanal production are modeled as presented in previous hydroformylation processes. In this case, the operating conditions for producing heptanal have been taken from the Union Carbide patent.[62] The process is suggested to operate at 90 ºC and with a pressure of ~25 bar with a syngas to olefin ratio of 3:1 and a H_2:CO ratio of 1:1 under Rhodium catalysts. The conversion achieved per pass is reported to be 88%, so unreacted raw materials are separated from aldehydes and recovered. A summary of the consumptions and correlation for the estimation of the CAPEX are given in Tables S-29, S-30, and S-31.

Table S-29. Summary of consumptions and function for CAPEX estimation for the production of heptanal.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	160.3415118	0.0207	0.1187
Heat (kcal/kg)	0		
Power (kJ/kg)	57.44000479		
CO (kg/kg)	0.1299827		
H2 (kg/kg)	0.0103986		

Table S-30. Summary of consumptions and function for CAPEX estimation for the production of octanal.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	136.861407	0.0283	0.808
Heat (kcal/kg)	0		
Power (kJ/kg)	58.9067		
CO (kg/kg)	0.095987		
H2 (kg/kg)	0.007578		

Table S-31. Summary of consumptions and function for CAPEX estimation for the production of nonanal.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	74.88614	0.0225	0.0701
Heat (kcal/kg)	0		
Power (kJ/kg)	36.547240		
CO (kg/kg)	0.0603436		
H2 (kg/kg)	0.0054858		

Oligomerization to higher carbon fractions

Fractions of olefins above C8 are assumed to be oligomerized for producing olefins with chains with more than 8 carbons that can be straightforwardly sold as lube oil or used in producing LAB, a surfactant. The process only includes the oligomerization section of alpha olefins presented in Figure S-12. A summary of the consumptions and CAPEX is provided in Table S-32.

Table S-32. Summary of consumptions and function for CAPEX estimation for the oligomerization of alpha olefins.

Type	Consumption	CAPEX	
		a	b
Ref (kcal/kg)	361.78273		

Heat (kcal/kg)	467.57791	0.0182	0.4081
Power (kJ/kg)	3.0760382		

Selective Separation of olefins and paraffins

One additional alternative considered is the separation of the olefins (hexene, heptene, octene) for their use as solvents or plasticizers. The separation of the olefins from paraffins is assumed to be carried out with the same consumptions as for pentene.

S-1.10.9 Power production

Light fractions (<C4) can also be burned to produce power sold to the power network. A Brayton cycle using a gas turbine is considered for generating power from gases. The summary of the CAPEX is provided in Table S-33. The CAPEX is estimated as a function of the power generated. No other OPEX is considered in the operation of the Brayton turbine. Power is computed as a function of the Brayton cycle efficiency and the LHV of the fuel burned as described in Eq. (S-9).

$$W = \eta_{Brayton} \sum_{i=1}^{i=Products} LHV_i \cdot F_i \tag{S-9}$$

Table S-33. Summary of consumptions and function for CAPEX estimation for the production of power by burning light paraffins.

CAPEX=a*W[MW]^b	
a	**b**
$1.8374 \cdot 10^6$	0.5889

S-1.10.10 Reforming of light olefins and paraffins.

A last alternative considered for the use of paraffins. The conversion of all the products is assumed to be the same as for methane. The energy required in the reforming process is assumed to be only the one in the difference of formation enthalpies between the CO and H_2 generated, and the formation enthalpy of the raw material. It is assumed that the energy required in heating the inlet to 950 ºC is integrated with the hot inlet, leaving the reactor that needs to be cooled down. The Capex is estimated as for methane, where with the parameters of Table S-34.

Table S-34. Summary of function for CAPEX estimation for the reforming of light paraffins.

CAPEX=a*W[MW]^b	
a	**b**
0.0219	0.864

S-1.11 Chemical recycling for recovery of LDPE from multilayer plastics.

A last alternative considered is the selective recovery of the polymer after its extraction from a multilayer plastic. In the process that we have modeled, we focus on the recovery of the LDPE presented in multilayer plastics. Toluene is initially employed for dissolving PE and then, acetone is employed as an antisolvent for isolating the PE. Finally, toluene is separated from acetone by distillation and recycled.[66] The process is presented in Figure S-34. After recovering PE, it needs to be sent to an extruder. Since the extruder is not available in Aspen Plus, it is computed offline. A summary of the consumptions and the parameters of the CAPEX function are given in Table S-35.

Table S-35. Summary of consumptions and function for CAPEX estimation for the recovery of PE with the solvent-antisolvent process.

Type	**Consumption**	**CAPEX**	
		a	**b**
Ref (kcal/kg)	86.7	0.0204	0.9305
Heat (kcal/kg)	84		
Power (kJ/kg)	0		
Toluene (kg/kg)	0.0035		
Acetone (kg/kg)	0.017		

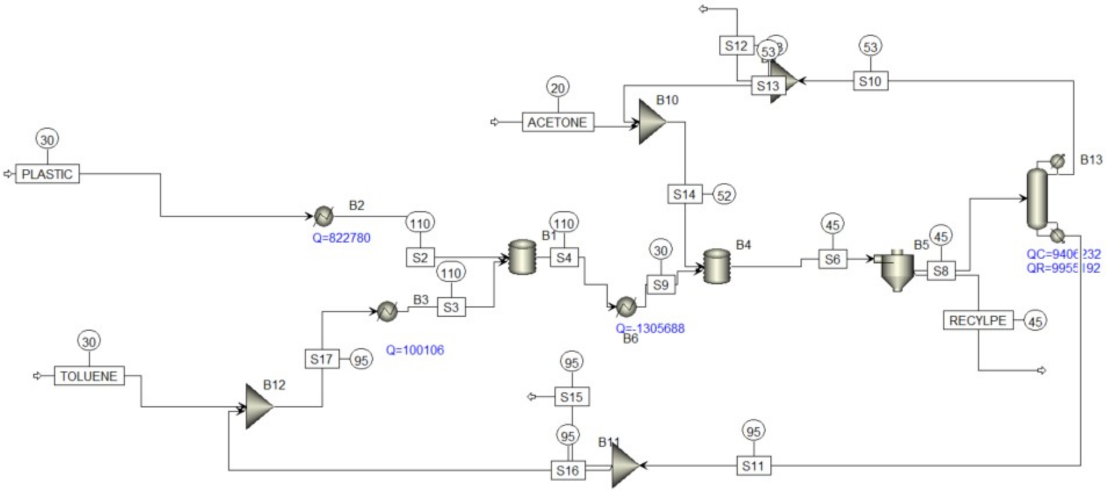

Figure S-34. Aspen process model for the selective separation of polyethylene from plastic waste. Note that an extruder is necessary after PE is separated from the plastic waste.

S-2. GENERAL ASSUMPTIONS IN THE TECHNOECONOMIC ANALYSIS.

The following assumptions are considered in the estimation of the OPEX and CAPEX in the superstructure:

- The recovery period of the CAPEX of the plants is assumed to be 10 years.
- Costs are determined based on the 2021 price basis. The costs are updated to 2021 with the Chemical Engineering Plant Cost Index of the Chemical Engineering journal.[67]

- The estimation of the CAPEX of the entire facility including yard, piping, electrical installation, contracts, etc. is determined from the cost of the main components of the process following the factors provided in Peters and Timmerhaus.[5]
- The cost employed in the prices obtained for products, raw materials, and utilities are summarized with their references in Table S-36.
- The utilities are assumed to cost \$7/MMBTU for natural gas, \$0.072/kWh for electricity, and \$2.1/ton for refrigerating water. The efficiency of natural gas furnaces is 75%, and the efficiency in generating steam in a boiler is 85%. The electricity is supplied directly. Water is assumed to be internally recycled in the refinery, with losses in the refrigeration tower estimated at 10%. A temperature difference of 10 ºC is assumed in the refrigeration circuit.

Table S-36. Summary of components, costs, and their references.

Component	**Price**
Heat from Nat Gas[68]	\$6.6/MMBTU
Electricity[69]	\$0.072/kWh
Refrigeration water[70]	\$2.1/ton
Ferric chloride in pretreatment[2]	0.538 (\$/kg)
NaOH[71]	0.626 (\$/kg)
Polyelectrolyte, starch[72]	0.725 (\$/kg)
Low Density Polyethylene (non-degraded)[73]	1.38 (\$/kg)
Natural gas[68]	6.6 (\$/MMBTU)
Propane[74]	2.983 (\$/gal)
C5-C10 Paraffins as gasoline[75]	4.44 (\$/gal)
C11-C19 paraffins as Diesel[75]	5.57 (\$/gal)
>C20 paraffins as Jet Fuel[76]	6.95 (\$/gal)
Hydrogen[77]	2.1 (\$/kg)
Methanol[78]	0.529 (\$/kg)
Lube oil. [79]	1.6 (\$/kg)
LAB, Surfactants[80]	2.08 (\$/kg)
Acetaldehyde[81]	2.4 (\$/kg)
Ethanol[82]	0.998 (\$/kg)
Propanal, asummed as acetaldehyde	2.4 (\$/kg)
Ethylene oxide[83]	1.251 (\$/kg)
Polypropylene[84]	2.02 (\$/kg)
Butanal[85]	2.49(\$/kg)
Acetone[86]	1.1 (\$/kg)
Propanol, assumed as iso-propyl-alcohol[87]	1.662 (\$/kg)
Acrylonitrile[88]	1.525 (\$/kg)
HCN[89,90] (Updated with cost index from EPA report)	2.952 (\$/kg)
Acrylic acid[91]	1.523 (\$/kg)
Polybutylene[92]	2.125 (\$/kg)
Butanol[93]	2.252 (\$/kg)
SBR[94]	3.288 (\$/kg)
Pentanal, valeraldehyde	5.5 (\$/kg)
Hexanal to nonanal, as aldehydes for cyclic polymers[95,96]	8.5 (\$/kg)

Hexane and hexene (as separated fractions), solvents.[97]	2.158 ($/kg)
Heptane, heptene, octane and octene (as separated fraction)[98]	2.434 ($/kg)
Benzene used in LAB[99]	1.827 ($/kg)
Styrene used is SBR[94]	1.650 ($/kg)
NH3[100]	0.664 ($/kg)
Oxygen[101]	0.1 ($/kg)
Purified water[102]	0.03 ($/kg)

S-3. GENERAL ASSUMPTIONS IN THE LIFE CYCLE ASSESSMENT

Life Cycle Assessment (LCA) is performed to determine the uses of plastic waste that have the best environmental performance attending to two objectives: On the one hand, the study aims to determine the superstructure that has the highest decarbonization potential at 100 years measured as Global Warming Potential – 100 (GWP100). On the other hand, an objective function is defined to minimize the impact on the environment by minimizing the impact on the Ecosystems quality of the Recipe method.[103] In the estimation of these two indicators, the following approaches are considered:

- Emissions are only computed considering the fluxes of each of the processes. The construction of the facilities, the catalysts, and other fixed materials are not considered in the LCA study.
- System expansion method is used for computing the emissions. The products generated are substituted with an oil-based product as basis. The boundaries of the system are simplified in Figure S-35. In this system expansion approach, the products obtained from the plastic-based refinery design are substituted by petrol-based products. A summary of the products considered for substitution is given in Table S-37.
- All the emissions factors for the products substituted, raw materials, and utilities are taken from Ecoinvent, with the products used for substitution to be those given in Table S-37.

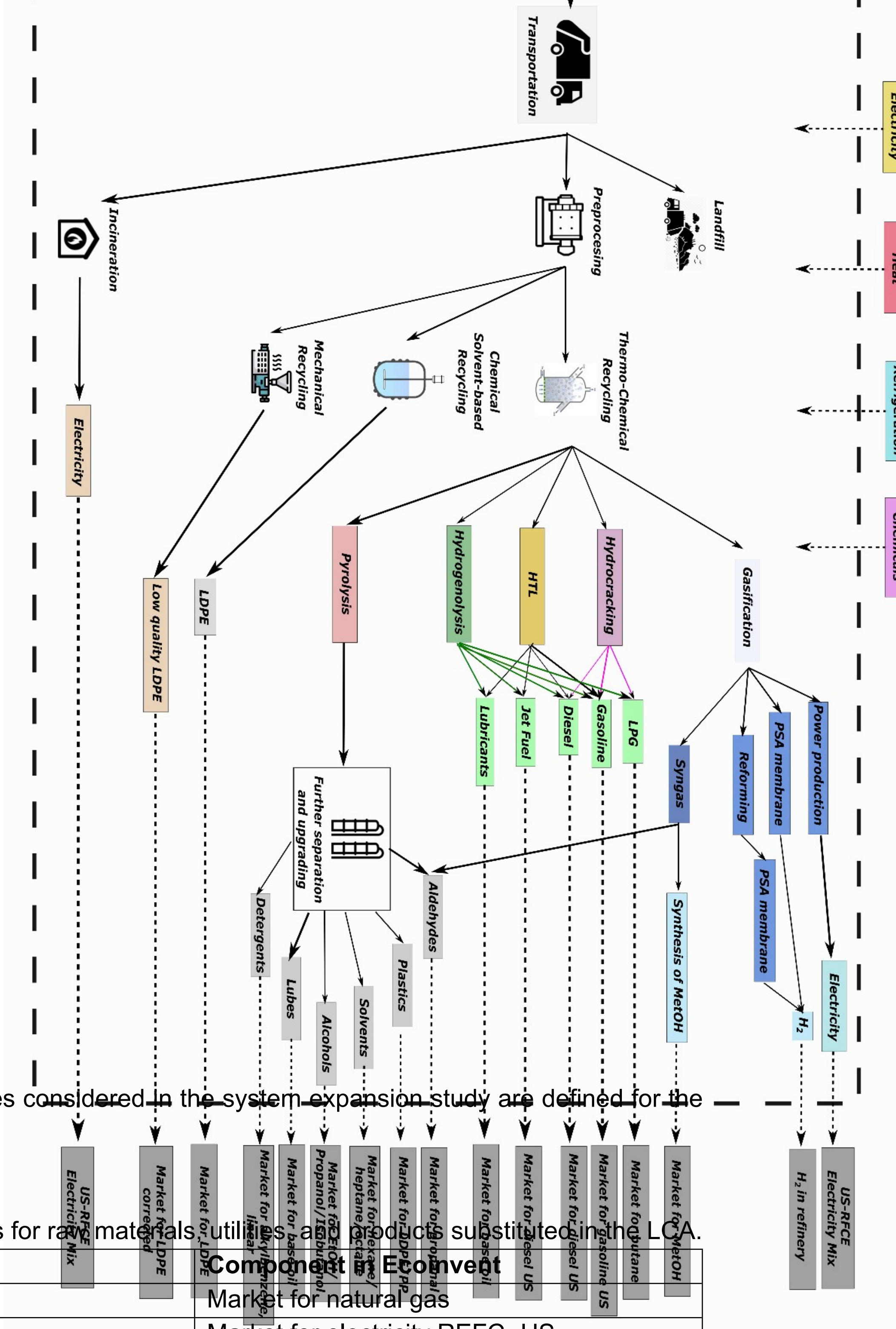

Figure S-35. Boundaries considered in the system expansion study are defined for the LCA.

Table S-37. References for raw materials, utilities, and products substituted in the LCA.

Component	**Component in Ecoinvent**
Heat from Nat Gas	Market for natural gas
Electricity	Market for electricity REFC- US
Refrigeration water	Market for tap water, Rest of the World
Ferric chloride in pretreatment	Iron (III) chloride production, without water, in 12% iron solution
NaOH	Market for sodium hydroxide, without water, in 50% solution state
Polyelectrolyte, starch	Maize starch production
Low Density Polyethylene (non-degraded)	Market for polyethylene, low density, granulate
Natural gas	Market for natural gas, high pressure, US
Propane	Market for propane
C5-C10 Paraffins as gasoline	Market for petrol, uleaded

C11-C19 paraffins as Diesel	Diesel production, petroleum refinery operation
>C20 paraffins as Jet Fuel	Diesel production, petroleum refinery operation
Hydrogen	Hydrogen production, gaseous, petroleum refinery operation
Methanol	Market for methanol
Lube oil.	Base oil production, petroleum refinery operation
LAB, Surfactants	Alkylbenzene production, linear
Acetaldehyde	Market for acetaldehyde
Ethanol	Ethanol production from maize
Propanal	Market for propanal
Ethylene oxide	Market for ethylene oxide
Polypropylene	Market for polypropylene, granulate
Butanal	Hydroformylation of propylene
Acetone	Market for acetone, liquid
Propanol, assumed as iso-propyl-alcohol	Isopropanol production
Acrylonitrile	Sohio process, acrylonitrile
HCN (Updated with cost index from EPA report)	Hydrogen cyanide production
Acrylic acid	Acrylic acid production
Polybutylene	Market for butene
Butanol	2-butanol production by hydration of butene
SBR	Latex production.
Pentanal, valeraldehyde	Hydroformylation of butene
Hexanal to nonanal, as asldehydes for cyclic polymers	**Assumed as hydroformylation of butene.
Hexane	Market for hexane
Heptane	Market for heptane
Octane	**Assumed as heptane.
Hexene	**Assumed as hexane
Heptene	**Assumed as heptane
Octene	**Assumed as heptane
Benzene used in LAB	Benzene production
Styrene used is SBR	Market for styrene
NH_3	Market for ammonia, anhydrous, liquid
Oxygen	Air separation, cryogenic, oxygen, liquid.
Purified water	Water production, ultrapure, US
Landfill operation	Treatment of waste plastic, mixture, unsanitary landfill, moist infiltration class (300 mm)

S-4. MODEL DESCRIPTION

S-4.1. Model formulation

All the surrogate models of the processes have been included in the MINLP optimization problem for selecting the optimal process attending to economic and GWP objectives. In the MINLP model, the processes are represented by two sets denoted as, *i* and *k*. The fluxes are represented by arcs between the sets of processes as $F_{i,k}$. The flux of each component getting into each of the processes, $f_{j,i,k}$ is employed for determining the outflow of the products as a function of the inflow of the principal reactant denoted by the index *"react"* getting into the process *k,* see (Eq. S-10). The inert components are not assumed to react. The flow of raw materials consumption, $f_{raw\,mat}$, is also determined as given in Eq. (S-11) as a function of the principal reactant *"react"* multiplied by a parameter, $a_{raw\,mat}$. The utilities consumption is determined as a function of the total inflow, $F_{i,k}$, get into each process *k*, multiplied by a parameter, a_{util},as given in Eq. (S-12).

$$f_{j,i,k} = yield_{react,\ j} \cdot f_{react,k} \tag{S-10}$$

$$f_{raw\,mat} = a_{raw\,mat} \cdot f_{react,k} \tag{S-11}$$

$$C_{util} = a_{util} \cdot F_{i,k} \tag{S-12}$$

Similarly, the Capex is computed for each of the units following a piecewise linear model with 5 cuts denoted by the index "z", implemented into the MINLP formulation as given in Eq. (S-13) to Eq. (S-17). The CAPEX of each of the units is computed as the sum of the CAPEX determined in each of the cuts, Eq. (S-13). In Eq. (S-13), Cap_z, corresponds to the CAPEX in each of the cuts and α_z is a positive continuous variable to select the value according to a flux. This selection of α_z is made based on the flux as given in Eq. (S-14), where the collocation points of the flux are given as γ_z. The sum continuous variables for selecting the collocation, α_z, must be restricted to 1, Eq. (S-15). Furthermore, it is necessary to implement the constrain that: at most two of the α_z must be positive. This is carried out by utilizing a binary variable, y_z that selects the α_z depending on the cut as given in Eq. (S-16). Eq. (S-17) indicates that only one region can be selected.

$$Capex_k = \sum_{z=1}^{z=5} Cap_z \cdot \alpha_z \tag{S-13}$$

$$F_{i,k} = \sum_{z=1}^{z=5} \gamma_z \cdot \alpha_z \tag{S-14}$$

$$\sum_{z=1}^{5} \alpha_z = 1 \tag{S-15}$$

$$\begin{aligned} &if\ z = 1: && \alpha_z \le y_z \\ &if\ 1 < z < 5: && \alpha_z \le y_z + y_{z-1} \\ &if\ z = 5: && \alpha_z \le y_{z-1} \end{aligned} \tag{S-16}$$

$$\sum_{z=1}^{5} y_z = 1 \tag{S-17}$$

Among the set of processes, the subset of separators is employed for dividing the stream and selecting the appropriate path among the different options. The multiple alternatives that can be selected are modeled employing a separation fraction, $f_{sep,l}$, that divides the flow into its multiple alternatives, *l,* as shown in Eq. (S-18). The sum of fractions must meet the condition of being equal to 1, as given in Eq. (S-19). Although the selection of multiple alternatives can be achieved with other formulations in the form of a MILP problem (e.g. Mc-Cormick formulation), this work aims to allow the system to select two or more technologies simultaneously. Since the number of separators employed is high and more than two options can be selected, an MINLP formulation has been used.

$$\sum_{l=1}^{unit} F_{l,k} = F_{i,l} \cdot f_{sep,l} \tag{S-18}$$

$$\sum_{l=1}^{units} f_{sep,l} = 1 \tag{S-19}$$

Apart from these specifications, the components produced in pyrolysis and gasification are tracked in downstream operations as component fluxes. The composition is introduced in the pyrolysis as a parameter set. This allows to compute the fluxes of each component. The fluxes of each component are tracked downstream. This can be done since there are no mixers to change the flow composition. Only the overall flux is computed downstream as given in Eq. (S-20). This overall flux is employed in computing the CAPEX as shown in previous Eq. (S-14).

$$F_{i,k} = \sum_{j=1}^{j=N_{comp}} f_{j,i,k} \tag{S-20}$$

S-4.1. Objective functions

The MINLP problem is optimized by employing two objective functions employing Baron as a solver. On the one hand, an economic objective function determines the superstructure that maximizes the profit, Eq. (S-21). The profit is defined as the income minus the costs, where the income is computed considering all the products produced as seen in Eq. (S-22). The costs are computed as the sum of the amortization costs computed from the CAPEX, plus the costs of the raw materials and utilities, see Eq. (S-23).

$$max(Profit) = \max(Income - Costs) \tag{S-21}$$

$$Income = \sum_{j=1}^{j \in Products} f_j \cdot P_j \tag{S-22}$$

$$Costs = \sum_{k=1}^{Units} W_k{\cdot}P_{power} + \sum_{k=1}^{Units} Q_k{\cdot}P_{heat} + \sum_{k=1}^{Units} Q_{k\,ref}{\cdot}P_{Ref} + \sum_{k=1}^{Units}\sum_{i}^{Raw\,Mat} f_{j,k}{\cdot}P_j + \sum_{k=1}^{Units} Capex_k \tag{S-23}$$

The environmental function, obtained from the LCA is employed for minimizing the GWP or the impact on the Ecosystems quality, see Eq. (S-24). The LCA follows a system expansion approach, and it considers two terms: the emissions generated by the continuous operation of the processes and the credits. The emissions generated are the sum of those generated by the utilities, raw material consumption, and the sorted plastic and are computed with the flows multiplied by an emission factor Eq. (S-25). The credits are computed similarly, with the flows obtained for the products.

$$GWP = Emissions - Credits \tag{S-24}$$

$$Emissions = \sum_{k=1}^{Units} W_k{\cdot}GWP_{power} + \sum_{k=1}^{Units} Q_k{\cdot}GWP_{heat} + \sum_{k=1}^{Units} Q_{k\,ref}{\cdot}GWP_{Ref} + \sum_{k=1}^{Units}\sum_{Raw\,Mat=1}^{Raw\,Mat} f_{raw\,Mat}{\cdot}GWP_{raw,mat} + GWP_{LDPE} \tag{S-25}$$

$$Credits = \sum_{j=1}^{j\in Products} f_j{\cdot}GWP_j \tag{S-26}$$

S-5 RESULTS FROM THE COMPARATIVE ANALYSIS BETWEEN MECHANICAL RECYCLING AND CHEMICAL RECYCLING BASED ON SOLVENTS

S-5.1 Results for the multi-objective optimization with economic and environmental objectives.

In the following lines, the economic and environmental results obtained from the multi-objective optimization are presented. These points correspond to the points generated by the ε-constraint method between the best economic objective and the environmental objective. Furthermore, the technologies selected and a summary of the economic and environmental breakdown are provided.

Table S-38. Economic and environmental results obtained in the Pareto frontier.

Point Pareto	Profit (\$/s)	GWP (kg$_{CO2eq.}$/s)
1	3.097	-0.953
2	2.803	-1.314
3	2.649	-1.144
4	2.495	-1.504

5	2.341	-1.455
6	2.187	-1.617
7	2.034	-1.655
8	1.88	-1.794
9	1.735	-1.882
10	1.572	-1.763

Table S-39. Depolymerization technologies selected.

Point Pareto	Fraction to solvent-based recycling	Fraction to pyrolysis
1	0	1
2	0	1
3	0.0198	0.9802
4	0.0574	0.9425
5	0.3376	0.6623
6	0.4524	0.5475
7	0.6435	0.3365
8	0.7485	0.2515
9	0.9901	0.0109
10	1	0

Table S-40. Detailed description of technologies selected for pyrolysis in the points of the Pareto.

Point	C1	C2	C3	C4	C5	C6	C7	C8	>C8
1	Nat gas	Isomeriz	Isomer.	Isomer (55.7%), Hydrof. (44.3%)	Hydroformylation				Olig
2	Nat gas	Wacker	Acetone	Isomer (55.0%), Hydrof. (45%)	Hydroformylation				Olig
3	Nat Gas	Isom (88%) Aceton (12%)	Acetone	Isomer (41.0%), Hydrof. (59%)	Hydroformyl			Ext. Dest	Olig
4	NG (59%) Power (41%)	Isom	Acetone	Isomer	Hydroformyl			Ext. Dest	Olig

5	Power	Wacker	Isom	Hydroformyl			Olig
6	Power	Isom	Acetone	Hydroformyl		Ext. Dest	Olig
7	Power	Isom	Isom	Hydroformyl			Olig
8	Power	Isom	Acetone	Isom	Hydroformyl	Ext. Dest	Olig
9	Power	Isom	Hydrof	Polybut	Hydroformul		Olig
10	Solvent-Antisolvent based recycling						

Table S-41. Detailed breakdown of the costs in the points of the Pareto.

	Costs ($/s)			**Income Products ($/s)**			
Point	**Utilities**	**Raw Mat**	**Amortiz**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	0.043	0.101	0.255	0.16	3.275	0.193	-
2	0.044	0.061	0.259	0.157	2.470	0.180	-
3	0.038	0.054	0.230	0.156	2.505	0.171	0.034
4	0.041	0.052	0.224	0.127	1.798	0.112	0.101
5	0.025	0.046	0.182	0.025	1.626	0.183	0.595
6	0.029	0.065	0.187	0.022	1.278	0.128	0.798
7	0.012	0.034	0.112	0.013	0.828	0.059	1.135
8	0.010	0.043	0.091	0.084	0.412	0.012	1.320
9	0.000699	0.024	0.022	3.94e-5	2e-3	0	1.746
10	0.000062	0.031	0.012	-	-	-	1.764

Table S-42. Detailed breakdown of LCA results in the points of the Pareto.

	Emissions (kgCO2eq./s)			**Credits (kgCO2eq./s)**			
Point	**Power**	**Heat**	**Raw Mat**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	0.22037	0.1222	0.463	0.1228	1.634	0.473	-
2	0.21946	0.1284	0.400	0.1228	1.161	0.778	-
3	0.19847	0.1059	0.352	0.1217	1.201	0.442	0.037
4	0.20939	0.1208	0.314	0.1066	0.977	0.360	0.108
5	0.12834	0.0706	0.267	0.0819	0.824	0.379	0.636
6	0.15229	0.0847	0.222	0.0650	0.557	0.401	0.853
7	0.07022	0.0354	0.150	0.0105	0.416	0.270	1.214
8	0.06169	0.0322	0.108	0.0065	0.177	0.401	1.411
9	0.01734	0.0059	0.048	3.07e-5	8.30E-04	0.086	1.867
10	0.01698	0.0010	0.033	-	-	-	1.886

S-5.2 Results for the multi-objective optimization limiting the system to conventional technologies.

Table S-43. Economic and environmental results obtained in the Pareto frontier with conventional technologies.

Point Pareto	Profit ($/s)	GWP ($kg_{CO2eq.}$/s)
1	1.401	-0.3348
2	1.367	-0.456
3	1.333	-0.5222
4	1.298	-0.5894
5	1.264	-0.6592
6	1.229	-0.7318
7	1.195	-0.8035
8	1.161	-0.869
9	1.126	-0.9442
10	1.092	-1.0795

Table S-44. Depolymerization technologies selected.

Point Pareto	Fraction to mechanical recycling	Fraction to pyrolysis
1	0	1
2	0.089	0.911
3	0.185	0.815
4	0.282	0.718
5	0.374	0.626
6	0.489	0.511
7	0.594	0.406
8	0.310	0.690
9	0.800	0.200
10	1	0

Table S-45. Detailed description of technologies selected in the points of the Pareto with conventional technologies.

Point	C1	C2	C3	C4	C5	C6	C7	C8	>C8
1	Nat. Gas.	Isom	Isom	Hydroform.			Extract. Distill	Hydroform	Olig

2	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
3	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
4	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
5	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
6	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
7	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
8	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
9	Nat. Gas.	Isom	Isom	Hydroform.	Extract. Distill	Hydroform	Olig
10	Mechanical Recycling						

Table S-46. Detailed breakdown of the costs in the points of the Pareto with conventional technologies.

	Costs ($/s)			**Income Products ($/s)**			
Point	**Utilities**	**Raw Mat**	**Amortiz**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	0.03	0.027	0.150	0.1695	1.113	0.3255	0
2	0.027	0.027	0.140	0.1695	0.904	0.3895	0.0534
3	0.025	0.024	0.132	0.1335	0.809	0.3665	0.111
4	0.021	0.021	0.123	0.1335	0.712	0.3065	0.1692
5	0.012	0.018	0.113	0.117	0.611	0.273	0.2244
6	0.015	0.015	0.100	0.0945	0.507	0.2185	0.2934
7	0.012	0.012	0.089	0.075	0.403	0.175	0.3564
8	0.009	0.01	0.078	0.057	0.305	0.131	0.186
9	0.006	0.00567	0.065	0.036	0.198	0.087	0.48
10	8.4e-5	0	0.011	0	0.00E+00	1.25e-6	0.6

Table S-47. Detailed breakdown of LCA results in the points of the Pareto with conventional technologies.

	Emissions ($kg_{CO2eq./}$s)			Credits (kg_{CO2eq}./s)			
Point	**Power**	**Heat**	**Raw Mat**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	0.050	0.254	1.85E-01	0.1322	0.534	0.352	0
2	0.047	0.232	1.66E-01	0.1065	0.44	0.315	0.096
3	0.044	0.208	1.49E-01	0.1041	0.393	0.277	0.201
4	0.041	0.183	1.31E-01	0.1006	0.346	0.275	0.306
5	0.038	0.160	1.14E-01	0.0913	0.298	0.253	0.405
6	0.034	0.130	9.30E-02	0.0737	0.246	0.197	0.530
7	0.031	0.104	7.40E-02	0.0585	0.196	0.157	0.644
8	0.027	0.079	5.80E-02	0.0445	0.148	0.119	0.336
9	0.024	0.052	3.70E-02	0.0281	0.096	0.077	0.867
10	0.017	0.001	7.15E-05	0	0	0	1.084

Estimations for the different regions defined by the OECD employed for comparison.

The Pareto front with conventional and process intensification technologies has been compared with the current cost and emissions of the plastic waste management sites. The estimation of these costs and emissions has been performed employing previous correlations and the data from the OECD for different regions of the world.[104] The data contains the fraction of plastic waste sent to each of the management technologies and the mismanaged fraction. This mismanaged fraction is assumed to have the same cost and emissions as the plastic going to landfills. As a result, the fractions sent to each technology are those reported in Table S-48.

Table S-48. Fraction of plastic waste sent to each technology in the OECD regions.

Region	**Fraction to mechanical recycling**	**Fraction to incineration**	**Fraction to landfill**
US	0.04	0.16	0.80
Canada	0.06	0.04	0.89
Other OECD America	0.10	0.005	0.885
OECD European	0.14	0.44	

Union			0.42
Other OECD Europe	0.08	0.23	0.69
OECD Oceania	0.07	0.12	0.81
OECD Asia	0.12	0.72	0.16
OECD Avg	0.09	0.29	0.62
China	0.13	0.24	0.63
India	0.13	0.04	0.83
Latin America	0.1	0.01	0.89
Middle East and North Africa	0.05	0.01	0.94
Other Africa	0.06	0.01	0.93
Other EU	0.065	0.03	0.905
Other Eurasia	0.05	0.015	0.935
Other non-OECD Asia	0.09	0.04	0.87

This fraction is used to determine the costs and emissions involved in each of the processes. The costs and emissions are determined with the models presented in previous sections for mechanical recycling, incineration, and landfill. To estimate the costs the following assumptions are made:

- Only the operating costs are considered. Since the location and number of plants cannot be determined with the current model, the capital costs are not included.
- Similarly, no other costs are involved in the estimation (e.g. labor costs, taxes, maintenance).
- All the costs employ the prices defined in the previous section. There is no geographical variation of the costs.

Similarly, the GWP in each of the locations is determined based only on the emissions involved in the operation of the process. The geographically specific emissions of each location have not been considered. The emissions involved in the collection of plastic waste and the distribution of the products are also not included. The results obtained for each of the locations for the profitability, value generated, and GWP are presented in Table S-49.

Table S-49. Estimation of costs and emissions for the different regions defined by the OECD.

Region	GWP (CO_{2eq}/kg_{LDPE})	Value Generated ($/$kg_{LDPE}$)
US	0.47523338	-0.01449
Canada	0.30873582	0.00801
Other OECD America	0.23300197	0.0499025
OECD Eunion	0.77798632	0.07928
Other OECD Europe	0.54660619	0.023135
OECD Oceania	0.41251496	0.01516
OECD Asia	1.16083416	0.05164
OECD Avg	0.62106297	0.031325
China	0.52257782	0.07413
India	0.25973522	0.07923
Latin America	0.24261113	0.049245
Middle East and North Africa	0.27978163	-0.002005
Other Africa	0.27234753	0.008245
Other EU	0.29491474	0.01286
Other Eurasia	0.2863527	-0.0021325
Other non-OECD Asia	0.28947162	0.03823

S-5.3 Evaluation with mechanical recycling.

In order to determine the maximum number of recycling loops that can make mechanical recycling more sustainable than solvent-based recycling sensitivity analysis was performed. In the sensitivity analysis, an increasing number of recycling loops that the material can resist is considered, see Table S-50. Since degradation per loop is lower with more cycles, the price also increases, see Table S-50. Recycling the LDPE more times also saves a higher fraction of emissions, Eq. (S-27). The evaluation of different values for the maximum number of loops does not select mechanical recycling until LDPE can resist 6 recycling loops of mechanical recycling. The results obtained for the Pareto with this limit of 6 recycling loops in mechanical recycling are presented in Tables S-51 to S-55.

$$Price_{Degraded\ LDPE} = \left(1 - \frac{1}{N_{Loops}}\right) P_{LDPE\ Virgin} \qquad \text{(S-27)}$$

Table S-50. Economic and environmental results obtained in the Pareto frontier.

Maximum	Price LDPE recovered	Credits LDPE Recovered

Number loops	(\$/kg$_{LDPE}$)	(kg$_{CO2}$/kg$_{LDPE}$)
2	0.9	1.08
3	1.199	1.44
4	1.35	1.62
5	1.44	1.728
6	1.596	1.8

Table S-51. Economic and environmental results obtained in the Pareto frontier with LDPE being recycled up to 6 times in mechanical recycling.

Point Pareto	Profit (\$/s)	GWP (kg$_{CO2eq.}$/s)
1	3.097	-0.953
2	2.957	-1.081
3	2.803	-1.314
4	2.649	-1.144
5	2.495	-1.504
6	2.341	-1.455
7	2.187	-1.617
8	2.034	-1.655
9	1.88	-1.794
10	1.735	-1.882
11	1.572	-1.763

Table S-52. Fraction sent to each depolymerization technologies selected.

Point Pareto	Fraction to mechanical recycling	Fraction to pyrolysis
1	-	1
2	-	1
3	-	1
4	0.05	0.95
5	0.11	0.89
6	0.33	0.67
7	0.467	0.553
8	0.73	0.26
9	0.97	0.034
10	0.999	0.001
11	1	0

Table S-53. Detailed description of technologies selected in the points of the Pareto with LDPE being recycled up to 6 times in mechanical recycling.

Point	C1	C2	C3	C4	C5	C6	C7	C8	>C8
1	Nat. Gas	Wacker (84%), Isom 16%	Isom	Isom (55%), Hydroform (45%)	Hydroform.				Lubes
2	Nat Gas	Wacker	Acetone (25%), Isom (75%)	Isom (45%) Hydrofrom (55%)	Hydrofrom.				Lubes
3	Nat. Gas	Wacker	Acetone	Isom (59%), hydroform (41%)	Hydrofrom.				Lubes
4	Nat. Gas	Isom	Isom (88%), acetone (12%)	Isom (41%), hydroform (59%)	Hydrofrom.			Ext. Distil	Lubes
5	Nat. Gas	Isom	Acetone	Isom	Hydrofrom.			Ext. Distil	Lubes
6	Nat. Gas	Wacker	Isom (41%), acetone (59%)	Hydroform.					Lubes
7	Power	Isom	Acetone	Isom (96%)	Hydroform			Ext. Distil	Lubes
8	Nat Gas	Isom	Isom	Hydroform.					Lubes
9	Power	Et. Oxide	Acetone	Isom	Hydroform.			Ext. Distil	Lubes
9	Power	Isom	Acetone	Polybutylene	Hydroform.				Lubes
11	Mechanical Recycling								

Table S-54. Detailed breakdown of the costs in the points of the Pareto with LDPE being recycled up to 6 times in mechanical recycling.

	Costs ($/s)	Income Products ($/s)

Point	Utilities	Raw Mat	Amortiz	Lubes	Aldehydes	Others	LDPE
1	0.043	0.072	0.255	0.16	3.468	0.133	-
2	0.043	0.066	0.263	0.16	3.327	0.127	-
3	0.044	0.038	0.259	0.157	3.15	0.147	0.079
4	0.038	0.083	0.230	0.156	2.776	0.122	0.175
5	0.041	0.052	0.224	0.117	2.71	0.115	0.526
6	0.025	0.068	0.182	0.255	1.906	0.114	0.526
7	0.029	0.065	0.187	0.025	1.809	0.107	0.745
8	0.012	0.05	0.112	0.013	0.887	0.076	1.165
9	0.01	0.043	0.091	0.008	0.624	0.045	1.548
10	6.9e-4	0.024	0.022	3.9e-4	2e-3	0.001	1.594
11	1.2e-4	0.002	0.012	0	0	0	1.596

Table S-55. Detailed breakdown of LCA results in the points of the Pareto with LDPE being recycled up to 6 times in mechanical recycling.

	Emissions ($kgCO_{2eq.}/s$)			Credits ($kgCO_{2eq.}/s$)			
Point	**Power**	**Heat**	**Raw Mat**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	0.220	0.122	0.397	0.351	1.432	0.473	-
2	0.223	0.126	0.409	0.123	1.314	0.688	-
3	0.219	0.128	0.400	0.123	1.161	0.770	-
4	0.198	0.106	0.352	0.122	1.2	0.401	0.09
5	0.209	0.121	0.314	0.287	0.777	0.588	0.198
6	0.128	0.071	0.267	0.020	0.824	0.281	0.594
7	0.152	0.085	0.222	0.197	0.557	0.491	0.8406
8	0.070	0.035	0.150	0.011	0.416	0.36	1.314
9	0.062	0.032	0.108	0.066	0.177	0.084	1.746
10	0.017	0.006	0.048	3.04E-05	8.30E-04	2.62e-5	1.7982
11	0.017	0.001	0.005	0	0		1.8

S-5.4 The role of scale.

The plant treating 1 kg/s of plastic waste, has been evaluated under a smaller (0.07 kg/s) and a larger (2.1 kg/s), to check if there is any effect on the technologies selected.

However, the technologies selected are the same. The results obtained are presented from Table S-56 to Table S-60 for 0.07 kg/s.

Table S-56. Economic and environmental results obtained in the Pareto frontier for a plant processing 0.07 kg/s.

Point Pareto	Profit ($/s)	GWP (kgCO2eq./s)
1	0.203	-0.066
2	0.193	-0.08
3	0.182	-0.09
4	0.172	-0.1
5	0.161	-0.106
6	0.151	-0.112
7	0.14	-0.118
8	0.129	-0.124
9	0.119	-0.131
10	0.108	-0.132

Table S-57. Fraction sent to each depolymerization technology for a plant processing 0.07 kg/s.

Point Pareto	Fraction to solvent-based recycling	Fraction to pyrolysis
1	0	1
2	0	1
3	0.129	0.871
4	0.171	0.829
5	0.343	0.657
6	0.528	0.471
7	0.643	0.357
8	0.828	0.171
9	0.9	0.1
10	1	0

Table S-58. Detailed description of technologies selected in the points of the Pareto for a plant processing 0.07 kg/s. Syngas employed in hydroformylation is partially covered from gasification where a fraction of plastic waste is suggested to be sent.

Point	C1	C2	C3	C4	C5	C6	C7	C8	>C8
1	Power	Isom	Acet	Hydroformylation					Olig

			(53%) Isom (43%)			
2	Power	Wacker	Acet (74%) Isom (26%)	Hydroformylation		Olig
4	N Gas	Isom	Acet (85%) Isom (15%)	Hydrof (84%) Isom (16%)	Hydroformylation	Olig
5	N Gas	PE	Acetone	Isom	Hydroformylation	Olig
6	N Gas	PE	Acetone	Isom	Hydroformylation	Olig
7	N Gas	PE	Acetone	Isom	Hydroformylation	Olig
8	N Gas	PE	Acetone	Isom	Hydroformylation	Olig
9	N Gas	PE	Acetone	Isom (85%) Hydrof (15%)	Hydroformylation	Olig
10	Solvent-based recycling					

Table S-59. Detailed breakdown of the costs in the points of the Pareto for a plant processing 0.07 kg/s.

	Costs ($/s)			**Income Products ($/s)**			
Point	**Utilities**	**Raw Mat**	**Amortiz**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	3.000E-03	7.000E-03	0.028	3.000E-03	2.240E-01	1.200E-02	0
2	3.000E-03	6.000E-03	0.026	3.000E-03	2.000E-01	2.300E-02	0
3	3.000E-03	6.000E-03	0.023	3.000E-03	1.690E-01	2.350E-02	0.016
4	2.000E-03	5.000E-03	0.022	2.500E-03	1.290E-01	3.400E-02	0.021
5	1.722E-03	2.723E-03	0.018	1.200E-03	1.020E-01	2.700E-02	0.042

6	1.364E-03	2.974E-03	0.013	7.500E-04	7.700E-02	1.850E-02	0.065
7	1.089E-03	2.000E-03	0.010	4.500E-04	6.100E-02	8.500E-03	0.079
8	5.394E-04	2.670E-03	0.006	1.500E-04	2.900E-02	4.500E-03	0.102
9	4.201E-05	1.000E-03	0.002	1.200E-08	1.700E-06	2.800E-07	0.111
10	4.213E-06	8.700E-08	0.001	0	0	0	0.123

Table S-60. Detailed breakdown of LCA results in the points of the Pareto for a plant processing 0.07 kg/s.

	Emissions (kg$_{CO2eq./}$s)			**Credits (kg$_{CO2eq./}$s)**			
Point	**Power**	**Heat**	**Raw Mat**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	1.548E-02	8.475E-03	3.20E-02	2.340E-03	2.240E-01	0.009	-
2	1.531E-02	8.730E-03	3.20E-02	2.340E-03	2.000E-01	0.033	-
3	1.359E-02	7.774E-03	2.80E-02	2.310E-03	1.690E-01	0.037	2.527E-04
4	1.293E-02	7.571E-03	2.20E-02	1.170E-03	1.290E-01	0.062	1.959E-03
5	1.046E-02	6.079E-03	1.70E-02	9.359E-04	1.020E-01	0.049	1.146E-02
6	7.942E-03	4.523E-03	1.40E-02	5.850E-04	7.700E-02	0.033	3.340E-02
7	6.236E-03	3.335E-03	1.30E-02	3.510E-04	6.100E-02	0.021	6.326E-02
8	3.558E-03	1.780E-03	8.00E-03	1.170E-04	2.900E-02	0.01	9.838E-02
9	1.189E-03	3.661E-04	3.00E-03	9.593E-08	1.900E-06	0.1339989	1.188E-01
10	1.189E-03	3.797E-05	1.55E-07	-	-	-	1.320E-

							01

S-5.5 Results employing impact on Ecosystems Quality as an indicator.

Sensitivity analysis was performed to employ a more general indicator that includes other impacts apart from GWP. The results obtained by minimizing the Ecosystems Quality of Recipe are given in Table S-61 to S-63. For all different points in the Pareto front, the same configuration for the economic and environmental objectives are obtained.

Table S-61. Economic and environmental results obtained in the Pareto frontier. Maximizing the profit and minimizing the impact on the Ecosystems Quality results in the same value and selects the same technology.

Point Pareto	Profit ($/s)	Impact Ecosystems Quality (Species·y/s)
Max Profit	3.067	-1.548e-8
Min Env. Impact	3.067	-1.548e-8

Table S-62. Detailed description of technologies selected. Note that in all the Pareto, the same selection of technologies is selected.

Point	C1	C2	C3	C4	C5	C6	C7	C8	>C8
1	Power	Isom	Isom	Aldehydes					Oligome
2	Power	Isom	Isom	Aldehydes					Oligome

Table S-63. Detailed breakdown of LCA results in the points of the Pareto front when the impact on the ecosystem is minimized as an environmental function. The results are given for one point since the other points

	Impact Ecosystem (Species·y/s)			Impact Ecosystem (Species·y/s)			
Point	**Power**	**Heat**	**Raw Mat**	**Lubes**	**Aldehydes**	**Others**	**LDPE**
1	3.588e-10	9.389e-10	2.61e-9	2.08-10	1.85e-8	6.59e-10	-

NOMENCLATURE

$a_{raw\ mat}$	Parameter employed to determine the raw material consumption from the main raw material in each process block.
a_{util}	Parameter employed to determine the utilities consumption from the main raw material in each process block.
α_z	Parameter employed to relate the flux with the capital cost.
Cap_z	Capital cost of a section of the piecewise linear model.
$CAPEX$	Capital costs.
$Costs$	Summatory of costs involved in the superstructure.
$Credits$	Credits generated by substituting the products from the superstructure.
$Emissions$	Emissions generated in all the processes.
E_{in}	Energy generated by incineration.
$F_{i,k}$	Overall mass flow rate between units i and k.
f_j	Mass flow rate of a component j.
$f_{j,\ k}$	Mass flow rate of a component j getting into a unit k.
$f_{j,i,k}$	Mass flow rate of a component j, in a stream between units i and k.
f_{LDPE}	Flux of LDPE.
$f_{sep,l}$	Fraction of material sent to each stream l in a separator.
GWP_{heat}	Global Warming Potential of heat.
GWP_j	Global Warming Potential of a component j.
GWP_{LDPE}	Global Warming Potential of Low density poly-ethylene.
GWP_{power}	Global Warming Potential of power.
$GWP_{raw,mat}$	Global Warming Potential of a raw material.
GWP_{Ref}	Global Warming potential of refrigeration.
GWP	Global Warming Potential.
$Income$	Income generated in the superstructure considering all the products.
LHV	Low Heating value.
N_{Loops}	Number of recycling loops.
OPEX	Operating expenses.
P_{heat}	Price of heat.
P_j	Unitary price of a component.
$P_{LDPE\ Virgin}$	Price of virgin polyethylene.
P_{power}	Price of power.
P_{Ref}	Price of refrigeration.
$Price_{Degraded\ LDPE}$	Price of degraded LDPE as a function of the number or recycling loops.
$Profit$	Overall profit obtained in the system.
Q_k	Heat consumption in a process k.
$Q_{k\ ref}$	Heat required in refrigeration in a process k.
Wk	Power consumption in a process k.
$W_{shredder}$	Power in the shredder.
$W_{prod\ incin}$	Power produced in the incineration process.
$yield_{react,\ j}$	Parameter employed as yield in a product generation from the main reactant.
y_z	Binary variable in each of the cuts of the piecewise linear model.

α_z	Alpha variable employed in the piecewise linear model.
η_{incin}	Efficiency in the incineration process.
γ_z	Collocation points of the flux in the piecewise linear model.

Subscripts

Heat	Referred to the heat.
i	Set of processes.
j	Set of components in a stream.
k	Set of processes.
l	Set of process alternatives in a separator.
LDPE	Referred to the low density poly-ethylene.
Power	Referred to the set of power.
Raw mat	Referred to the raw material.
React	Referred to the main reactant.
Ref	Referred to the refrigeration.
Sep	Referred to the separators, set of separators.
Util	Referred to the utilities.
z	Set of cuts of the piecewise linear model.

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