

# Economic Evaluation of Infrastructures for Thermochemical Upcycling of Post-Consumer Plastic Waste Supplementary Information

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This supplementary information contains 21 pages and 5 sections and provides details on our overall methodology and case study. All scripts and data needed for reproducing the results are available at [https://github.com/zavalab/JuliaBox/tree/master/Plastic\\_value\\_chain](https://github.com/zavalab/JuliaBox/tree/master/Plastic_value_chain).

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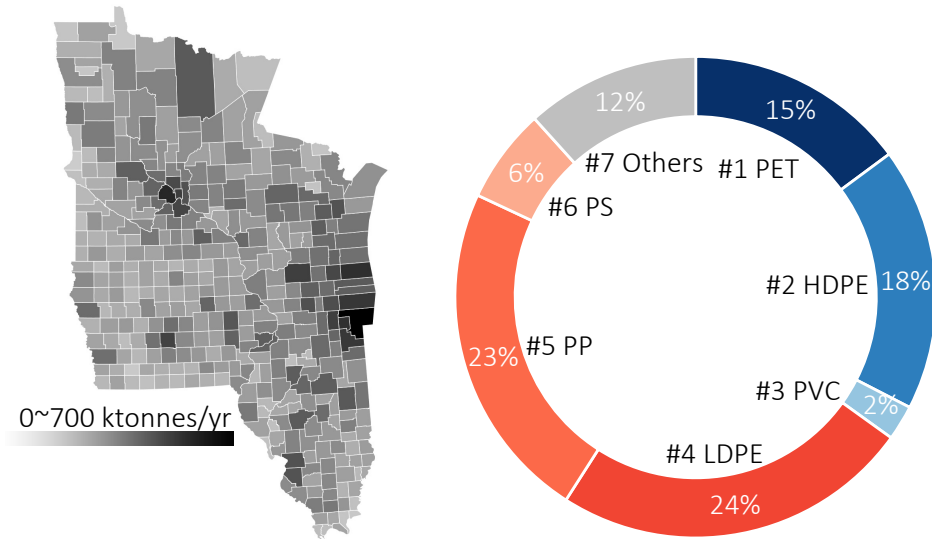
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# 1 Plastic Waste Characteristics

Law and co-workers estimated the US annual, per-capita plastic waste production in 2016 to be 130 kg [20]. We use this for estimating plastic waste generation at the county scale (multiplying the per-capita estimate by the county population gives the distribution). In taking this approach, we have implicitly assumed that the composition of plastic waste does not vary throughout the study area and is identical to the national average (reported by the US Environmental Protection Agency). We acknowledge that there are strong regional variations of plastic waste composition, but obtaining detailed data (at a per-county resolution) is difficult; we leave this as a topic of future work.



S-Figure 1: Plastic waste distribution in the upper Midwest region of the US (left) and post-consumer plastic waste composition obtained from the US EPA (right) [15, 7].

S-Table 1 presents the average post-consumer plastic waste composition in the US (reported by the US Environmental Protection Agency). Here, we can see that this is a complex mixture that is dominated by LDPE, PP, PET, and HDPE. PET and HDPE are typically recycled using mechanical pathways; as such, we target technologies to process plastic waste to produce the next dominant plastic types, LDPE and PP (thus creating a circular economy).

S-Table 1: Plastic waste composition reported by the US Environmental Protection Agency [15].

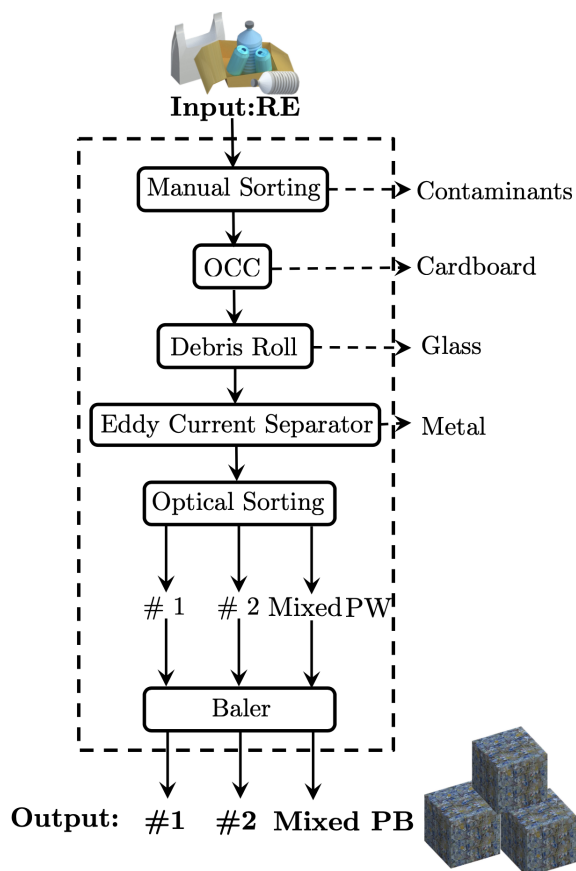
Plastic Type	Percentage (mass %)
#1 PET	15
#2 HDPE	18
#3 PVC	2
#4 LDPE	24
#5 PP	23
#6 PS	6
#7 Others	12

## 2 Plastic Waste Processing Technologies

In this section, we review the technologies comprising our plastic upcycling infrastructure. We provide schematic diagrams for each technology and highlight the major components of each process. In this work, the material and energy balances and cost data of processing facilities were first extracted from literature or provided by our industrial collaborators. Given the material and energy balance data of processing facilities, we derive the data needed for conducting techno-economic analysis and life-cycle assessment of the upcycling infrastructure. These data include yield factor, capital investment, operational cost and CO<sub>2</sub> emissions of technologies.

### 2.1 Materials Recovery Facility (MRF)

S-Figure 2 illustrates a typical materials recovery facility (MRF). MRFs are involved in the collection and sorting of municipal waste, producing bales of sorted products that are sold on to be recycled or for final disposal (e.g., incineration or landfilling). Our focus here is on MRF steps related to plastics separation and baling.



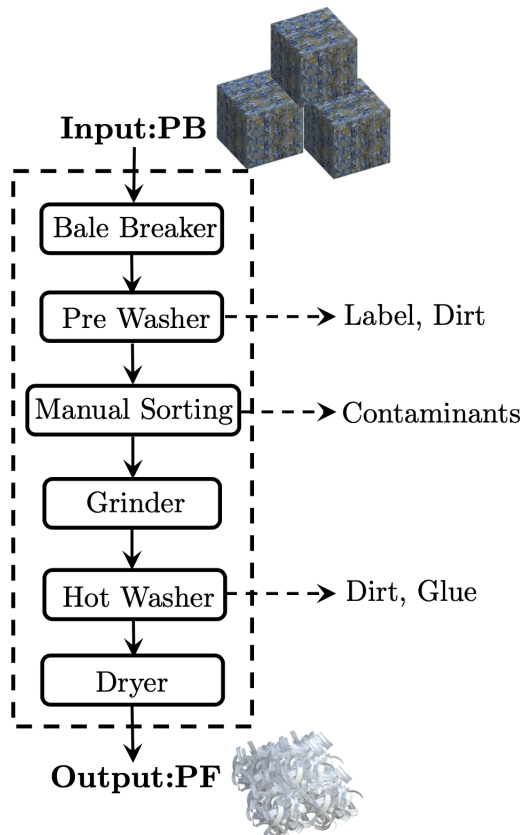
S-Figure 2: Simplified process flow sheet diagram of materials recovery facility (MRF) [26]

Waste haulers are the first element of the process, transporting materials to the MRF. The recyclables collection cost is estimated at 4.78 USD/tonne of recyclables [26]. The recyclables collection cost is reflected in the operational cost of MRF. Recyclable waste is a highly complex mixture,

and must be sorted to separate paper, glass, metal, and plastics. This separation is labor- and cost-intensive. Trucks dump mixed waste on the MRF tipping floor, where it is loaded onto conveyors. Workers remove any non-recyclable contaminants manually. Additionally, any recyclables that could damage the MRF equipment are removed as well (typically including bulky materials, scrap metal, or rope).

The remaining unsorted recyclables are transferred to old corrugated cardboard (OCC) screen, where several rotating disks separate cardboard. Remaining recyclables continue to the debris roll screen, which separates glass items. The glass is broken down into small shards by this process. Finally, an eddy current separator removes aluminum and iron materials using a magnetic field. The remaining stream comprises mixed plastics.

MRF operators separate #2 plastics (HDPE) manually; the remaining plastics are sent through an optical sorter, which uses light-scattering and spectrometry to separate plastics into groups by their resin types. Usually, #1 plastics are grouped for mechanical recycling, #2 plastics form a second group, and #3-#7 and non-bottle #1 and #2 plastics are grouped as mixed plastic waste. These separated plastic streams are baled and sent on to plastics reprocessing facilities (PRFs).



S-Figure 3: Simplified process flowsheet diagram of plastic reprocessing facility (PRF) [26, 9]

## 2.2 Plastic Reprocessing Facility (PRF)

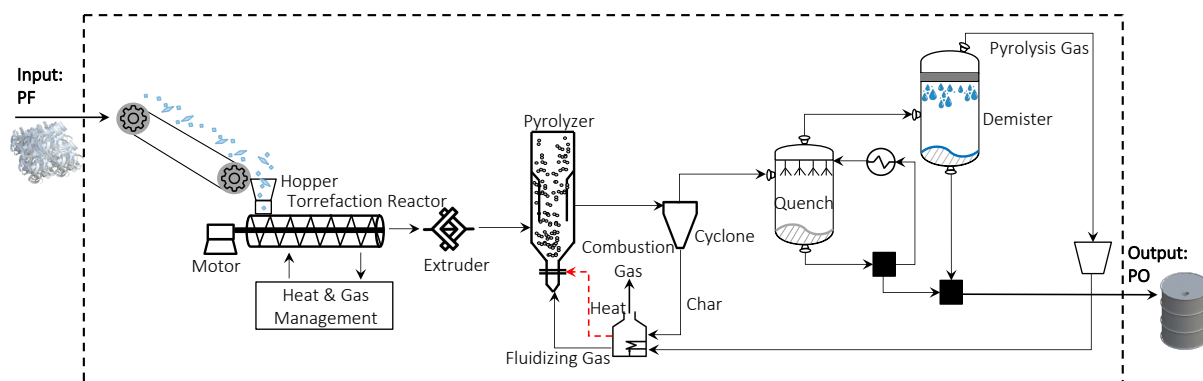
Plastics reprocessing facilities (PRFs) are a key connection between waste plastic and new materials. Specifically, these technologies convert the plastics sorted and baled at MRFs into a plastic flake product that is sold as a product; as such, they provide capabilities for ensuring that plastic waste is a suitable feedstock for other technologies (e.g., remove impurities and manipulate size to facilitate flow). Removing impurities is key for mechanical recycling and chemical upcycling.

S-Figure 3 illustrates the major processing steps involved at a PRF. Plastic bales delivered from an MRF are broken up by a bale breaker. From here, here the plastics are conveyed to a prewashing station where labels and dirt are removed. Manual sorting follows to remove any contaminants. Finally, the plastic is ground into small flakes and is washed one last time to remove any residual dirt or other impurities (e.g., adhesives).

## 2.3 Pyrolysis Process

Pyrolysis oil is produced from plastic flakes (which is a mixture of plastic types) by high-temperature decomposition under anoxic conditions. Figure 4 presents a schematic of a pyrolysis system considered here. Pyrolysis reactions are sensitive to the presence of certain chemicals, specifically chlorine (it both damages the equipment and reduces the quality of the pyrolysis oil) which means special pretreatment steps are required in order to process PVCs (thus adding cost) [22, 35, 33].

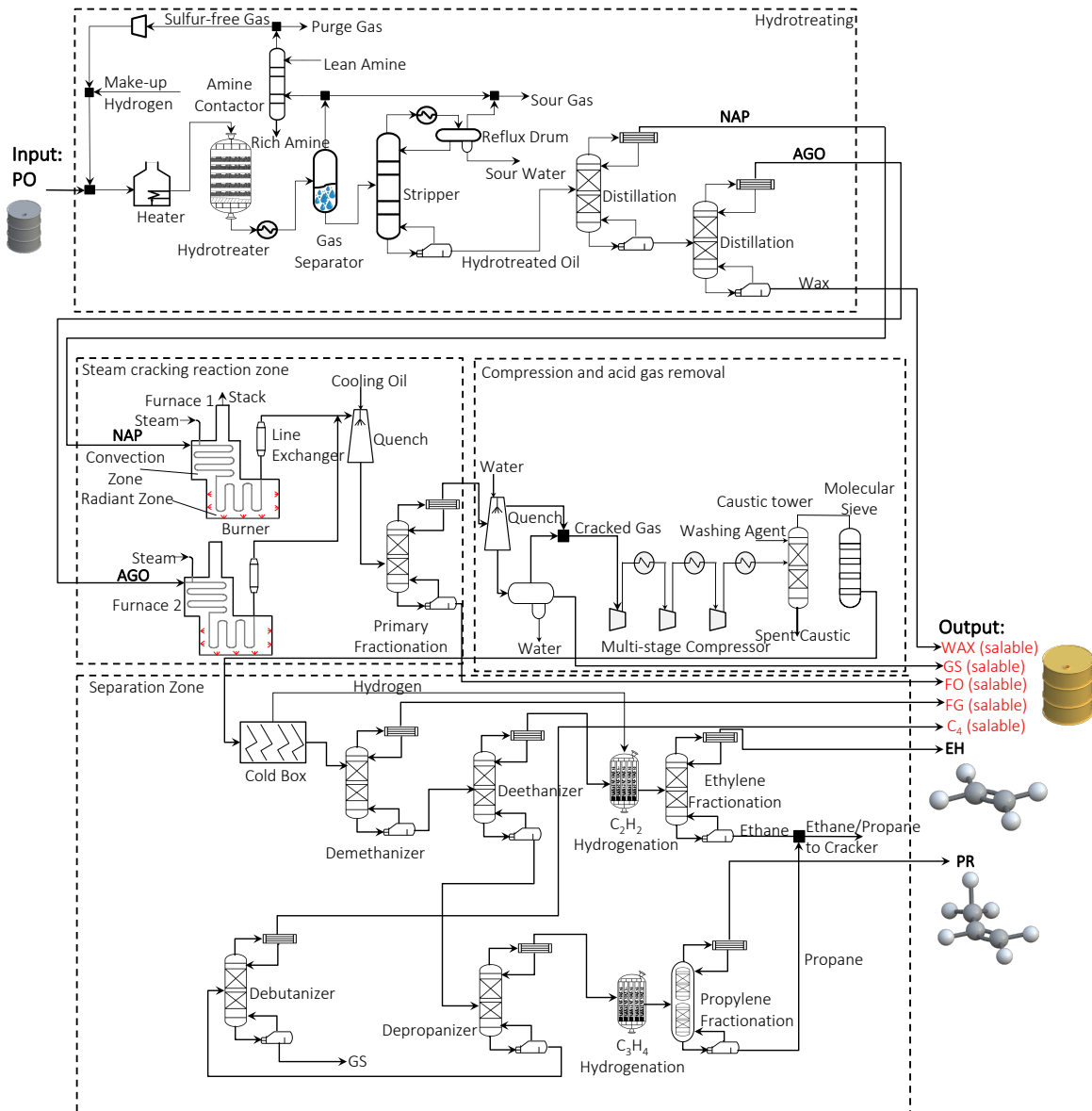
Plastic flakes brought to a pyrolysis facility are first run through a torrefaction reactor with an auger; this reactor is typically run at 300°C, and decomposes PVCs into ethylene and gaseous hydrochloric acid. Coupled to this reactor is a heat and gas management system that neutralizes the acidic gases with calcium hydroxide and provides reaction heat. The contents of the torrefaction reactor are a solid product and are extruded, then subsequently ground. The ground products are passed into the pyrolyzer proper, which is operated at 520°C, and converts the plastics into a mixture of gas, oil, and char[18]. The pyrolyzer products are sent to a cyclone that separates out pyrolysis char from the vapors. The vapor stream is quenched to condense the oils out of the vapor phase; remaining vapors passed through a demister to recover additional oil. A fraction of the recovered oil is recycled through the system as quenching fluid. Any remaining gases are recycled (along with the char) through a combustion process that provides heat and fluidization gases for the fluidizer.



S-Figure 4: Process flowsheet of pyrolysis system.

## 2.4 Steam Cracking Process

Steam cracking is a highly sophisticated process that converts pyrolysis oil into a variety of short-chain hydrocarbons that are suitable for industrial applications. In this section, we review the structure of a general steam cracking process. Pyrolysis oil, especially that produced from waste plastic, will fail to meet contaminant specifications for many downstream applications. Notable contaminants include nitrogen and sulfur, which are often present in the oil at unacceptable levels. Steam cracking is therefore preceded by hydrotreatment to reduce contaminant levels[19].



S-Figure 5: Process flowsheet of steam cracking facility (including hydrotreatment)[14, 21, 24].

One can find a schematic hydrotreatment process on top of S-Figure 5. Pyrolysis oil is fed into the system and mixed with hydrogen, preheated, and pumped into a hydrogenation reactor. This reaction yields a mixture of hydrotreated oil, light hydrocarbons, and off-gases, including hydro-

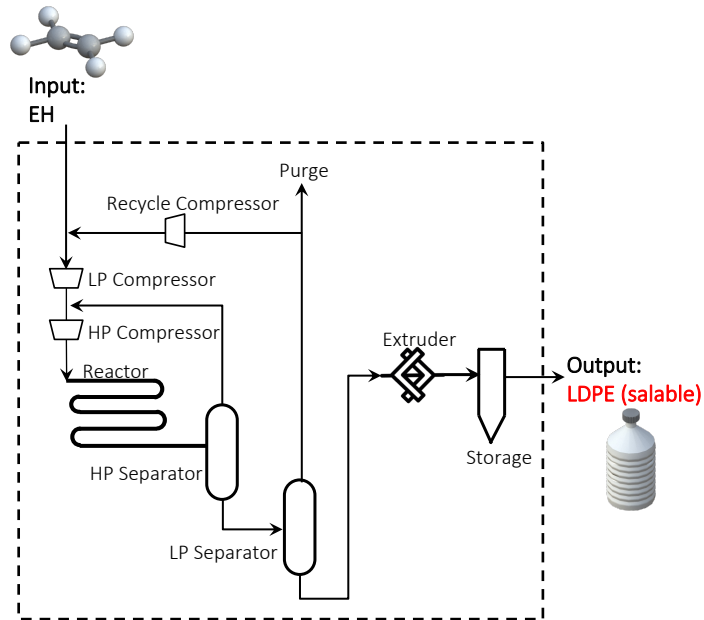
gen sulfide and ammonia. The reactor effluent is cooled and then flashed to separate the gases (including the hydrogen sulfide, ammonia, residual hydrogen, and any light hydrocarbons) from the hydrotreated oil. A gas separator passes these gases through an amine contactor to remove the hydrogen sulfide. With the contaminants removed, the hydrogen-rich gas is recycled back to the reactor.

The hydrotreated oil then passes through a stripper for further purification; the off-gases from this process are recycled along with the reactor off-gases. A purge stream ensures that sulfur does not accumulate in the system. The purge is typically treated by the Claus process to recover elemental sulfur. The oil stream undergoes distillations separating it into a naphtha fraction, a atmospheric gasoil (AGO) fraction and a wax fraction. In our models, the hydrotreatment process is incorporated with steam cracking.

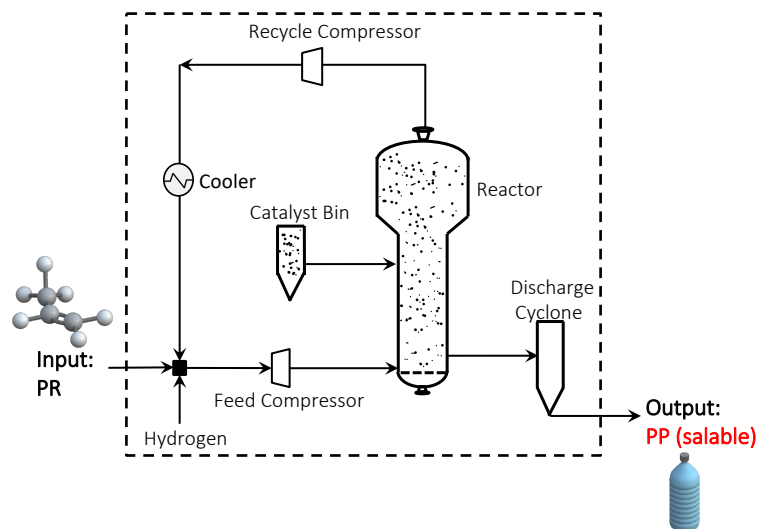
The steam cracking process is also outlined in S-Figure 5. The steam cracking process is divided into three sections, comprising the reactor, compression, and separation zones of the process. The first state of steam cracking is the cracking reaction, in which the naphtha and the AGO from the hydrotreater are fed to different furnaces and mixed with steam and heated using flue gas in the convection zone. This stream is heated to 500-680°C (the incipient cracking temperature). As the stream enters the tubular reactor the stream is heated up to 750-875°C in about 0.1-0.5 seconds. During this short residence time, the feed is cracked into smaller molecules, including ethylene, propylene, and other byproducts. Adding steam to the steam cracker facilitates the control of residence time, prevents coke formation, and reduces hydrocarbon partial pressure.

The effluent stream from the cracking furnaces is cooled by a transfer line exchanger (TLE) where feed water is vaporized and high-pressure steam is generated. Then the cracked gas is further cooled down by contacting with cooling oil in a quench oil tower. Subsequently, the cooled gas passes through the primary fractionation column, which separates fuel oil as its bottom product, and a top stream that passes through another round of quenching. Following this, the top stream goes through a three-phase separation producing water, liquid hydrocarbons, and gaseous hydrocarbons. The water is recycled back to the cracker, and the liquid hydrocarbon stream is collected as mixed pyrolysis gasoline. The gaseous streams from the quench process and three-phase separator are combined; this stream still contains valuable products that can be separated into relatively pure streams. The outlined separation process achieves this.

Following a round of multi-stage compression, CO<sub>2</sub> and H<sub>2</sub>S are removed by the caustic tower. Remaining water is removed by the molecular sieve dryer. The gas is cooled to -156°C in the cold box, under which condition hydrogen is separated from the stream. The recovered hydrogen is reserved for later hydrogenation processes. The gas stream is passes through four columns (the demethanizer, deethanizer, depropanizer, and debutanizer) with the bottom product from each passed to the next in order, culminating in the debutanizer bottom product, which is collected as pyrolysis gasoline. The separation top products are streams of methane, ethane, propane, and butane. The ethane and propane streams are independently hydrogenated to product ethylene and propylene (monomer products). The methane stream is recycle for heating, and residual ethane and propane are recycled.



S-Figure 6: Simplified process flowsheet diagram of polyethylene polymerization facility [8].



S-Figure 7: Simplified process flowsheet diagram of polypropylene polymerization facility [14].



## 2.5 LDPE and PP Polymerization Processes

LDPE polymerization proceeds according to the schematic in S-Figure 6. Purified ethylene at 99.9% purity is fed into the process. The feed is compressed to 150 - 300 MPa through by means of a two-stage compression system. Subsequently, the compressed feed is fed into a tubular reactor producing molten polyethylene. Two separators recover unreacted ethylene monomer. After one round of separation, the ethylene recycle is still under reasonable pressure and is reintroduced to the feed following the first compression step. The second separation process reduces the pressure further, and this stream is recycled back to the inlet, less a purge fraction. The polyethylene bottom product obtained from separation proceeds to extrusion and pelletization.

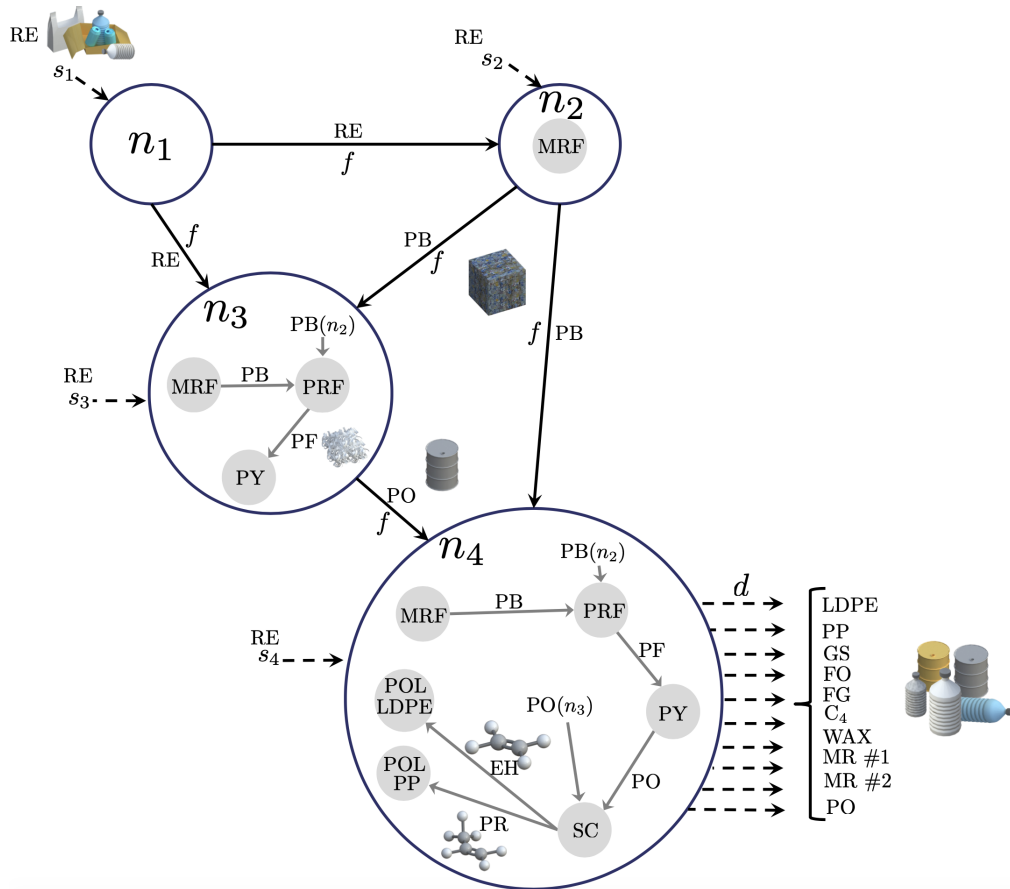
PP polymerization occurs in a fluidized bed reactor as shown in S-Figure 7. Propylene and hydrogen are thoroughly mixed in the dense-phase fluidized bed formed by Ziegler-Natta catalyst. The reactor is operated at a reaction condition as  $< 88 C^\circ$  and  $< 4$  MPa. The expanded upper section of the reactor(disengagement zone) enables the entrainment of catalyst. The recirculated gas is mixed with fresh feeding stream and is fed to reactor after a cooler removes reaction heat from it. A catalyst bin supplement the catalyst to the reactor constantly. Finally, the product PP powder and unreacted gas are separated using a discharge cyclone.

## 3 Infrastructure Optimization Formulation

We now formally introduce the optimization formulation used for designing upcycling infrastructures. As illustrated in S-Figure 8, we treat each county as a geographical node and use the node set  $\mathcal{N}$  to represent the 360 counties of the studied region. We consider each county as a plastic supplier and use set  $\mathcal{S}$  to denote the 360 plastic waste suppliers in the studied region. Each plastic supplier  $i \in \mathcal{S}$  has an associated plastic supply flow  $s_i \in \mathbb{R}_+$ , maximum supplying capacity  $\bar{s}_i \in \mathbb{R}_+$ , location  $n(i) \in \mathcal{N}$ , and offering price  $\alpha_i^s \in \mathbb{R}_+$ . For infrastructure layouts I, III, and IV, the plastic waste is provided in the form of mixed recyclables. For infrastructure layout II, since plastic is sorted by people in their households, suppliers provide a plastic waste mixture (plastic bale) directly.

The set of products (including raw materials, intermediate and final products) is denoted as  $\mathcal{P}$ . For infrastructure layout I, the product set is defined as  $\mathcal{P} := \{\text{recyclables, plastic bale, plastic flake, pyrolysis oil, ethylene, propylene, } C_4, \text{ pyrolysis gasoline, fuel gas, fuel oil, LDPE, PP, wax}\}$ . For infrastructure II, since the MRF is bypassed, the product set is defined as  $\mathcal{P} := \{\text{plastic waste, plastic flake, pyrolysis oil, ethylene, propylene, } C_4, \text{ pyrolysis gasoline, fuel gas, fuel oil, LDPE, PP, wax}\}$ . For infrastructure III, PET and HDPE bottles are mechanically recycled. Therefore, the product set is defined as  $\mathcal{P} := \{\text{recyclables, \#1 plastic bale, \#2 plastic bale, mixed plastic bale, mechanically recycled \#1 flake, mechanically recycled \#2, mixed plastic flake, pyrolysis oil, ethylene, propylene, } C_4, \text{ pyrolysis gasoline, fuel gas, fuel oil, LDPE, PP, wax}\}$ . For infrastructure IV, pyrolysis is the only thermochemical facility; therefore, the product set in this case is  $\mathcal{P} := \{\text{recyclables, plastic bale, plastic flake, pyrolysis oil}\}$ .

As shown in S-Figure 8, we have the set of consumers  $\mathcal{D}$  requesting final products (LDPE, PP, pyrolysis gasoline, fuel gas, fuel oil,  $C_4$ , wax,mechanically recycled #1, mechanically recycled #2



S-Figure 8: Schematic of infrastructure optimization problem highlighting complex interdependencies between products and technologies that arise from product transformation and geographical transport.

and pyrolysis oil). For each final product at each node, there is a corresponding consumer  $j \in \mathcal{D}$ . Each consumer has a demand flow  $d_j \in \mathbb{R}_+$ , requested product type  $p(j) \in \mathcal{P}$ , location of consumer  $n(j) \in \mathcal{N}$ , and product purchasing price  $\alpha_j^d \in \mathbb{R}_+$ . The products are requested at current market values of these products.

Technologies are indexed  $t \in \mathcal{T}$ . We denote the subset of technologies located in node  $n$  as  $\mathcal{T}_n \subseteq \mathcal{T}$ , with  $\mathcal{T}_n := \{t \in \mathcal{T} \mid n(t) = n\}$ . Each county is considered a potential location for the technologies. Therefore, the proposed plastic upcycling infrastructure comprises 360 potential sites for installing technology facilities. For infrastructure I and III, we have in total six technologies considered: MRF, PRF, pyrolysis, steam cracking, LDPE polymerization and PP polymerization. For infrastructure II, since MRF is bypassed, we have five technologies involved: PRF, pyrolysis, steam cracking, LDPE polymerization and PP polymerization. For infrastructure IV, there are only three technologies, including MRF, PRF and pyrolysis. Each technology is affiliated with yield factors  $\gamma_{t,p} \in \mathbb{R}$ , location  $n(t) \in \mathcal{N}$ , reference product  $p(t) \in \mathcal{P}$ , processing capacity  $\bar{\xi}_t \in \mathbb{R}_+$ , operating cost  $\alpha_t^\xi \in \mathbb{R}_+$ , number of facilities installed  $y_t \in \mathbb{Z}_+$ , annualized installation cost  $\alpha_t^y \in \mathbb{R}_+$ . Yield factors  $\gamma_{t,p} \in \mathbb{R}$  denote the units of product  $p$  consumed/generated per unit of reference product  $p(t)$  consumed/generated in a given technology  $t$  (e.g., how many units of pyrolysis oil can be produced from one unit of plastic flakes fed into the system); here,  $\xi_t \in \mathbb{R}_+$  is the amount of product  $p(t)$  processed at technology  $t$ . The yield factors, operating costs, installation costs, and capacities are key pieces of techno-economic data; obtaining this information requires conducting a detailed TEA for each technology and require experimental data (e.g., yield factors).

Transport providers are indexed as  $\ell \in \mathcal{L}$  with flow  $f_\ell \in \mathbb{R}_+$ , cost  $\alpha_\ell^f \in \mathbb{R}_+$ , product type transported  $p(\ell) \in \mathcal{P}$ , sending (origin) node  $n_s(\ell) \in \mathcal{N}$  and receiving (destination) node  $n_r(\ell) \in \mathcal{N}$ . As shown in S-Figure.8, to avoid transporting gaseous olefins, polymerization facilities are built with steam cracking facilities in the same location. Transportation providers only move recyclables (plastic waste in infrastructure II), plastic bale, plastic flake and pyrolysis oil cross nodes. These four products could be shipped cross any pair of nodes in the supply chain network. To simplify the notation for transport, we define  $\mathcal{L}_{n,p}^{in}$  as a subset of transportation provider  $\ell \in \mathcal{L}$  that sends product  $p$  to node  $n$ . Subset  $\mathcal{L}_{n,p}^{out}$  includes transportation provider that transports  $p$  away from  $n$ .

$$\max_{(s,d,f,\xi,y)} \sum_{j \in \mathcal{D}} \alpha_j^d d_j - \sum_{i \in \mathcal{S}} \alpha_i^s s_i - \sum_{\ell \in \mathcal{L}} \alpha_\ell^f f_\ell - \sum_{t \in \mathcal{T}} \alpha_t^\xi \xi_t - \sum_{t \in \mathcal{T}} \alpha_t^y y_t \quad (3.1)$$

$$\text{s.t.} \left( \sum_{i \in \mathcal{S}_{n,p}} s_i + \sum_{\ell \in \mathcal{L}_{n,p}^{in}} f_\ell \right) - \left( \sum_{j \in \mathcal{D}_{n,p}} d_j + \sum_{\ell \in \mathcal{L}_{n,p}^{out}} f_\ell \right) + \sum_{t \in \mathcal{T}_n} \gamma_{t,p} \xi_t = 0, (n,p) \in \mathcal{N} \times \mathcal{P} \quad (3.2)$$

$$s_i = \bar{s}_i, i \in \mathcal{S} \quad (3.3)$$

$$\xi_t \leq y_t \bar{\xi}_t, t \in \mathcal{T}. \quad (3.4)$$

The objective (3.1) is to maximize the total annual economic surplus (profit) of the plastic upcycling infrastructure. This is defined as value of product demands served minus supply, technology (processing), and transportation costs. Equation (3.2) ensures that each product  $p \in \mathcal{P}$  at each node  $n \in \mathcal{N}$  is in balance. Constraint (3.3) ensures that all the plastic waste is processed in the value chain. Constraint (3.4) imposes capacity bounds for each technology; the processing capacity of technology

is zero if the facility is not built ( $y_t = 0$ ); otherwise ( $y_t > 0$ ), the total capacity is given by the per facility capacity  $\bar{\xi}_t$  and the number of facilities built ( $y_t$ ). This optimization model is a mixed-integer linear program (MILP).

After solving the above MILP, we fix the integer variables  $y_t$  and this transforms the above MILP into a linear program (LP). This transformation is equivalent to having technologies already installed and thus only aims to find the best distribution of products across technologies that maximize the economic surplus. In other words, the goal is then is to optimize the plastic upcycling infrastructure with predefined number, size, and location of facilities (this simulates the operation of a value chain).

$$\max_{(s,d,f,\xi)} \sum_{j \in \mathcal{D}} \alpha_j^d d_j - \sum_{i \in \mathcal{S}} \alpha_i^s s_i - \sum_{\ell \in \mathcal{L}} \alpha_\ell^f f_\ell - \sum_{t \in \mathcal{T}} \alpha_t^\xi \xi_t \quad (3.5)$$

$$\text{s.t.} \left( \sum_{i \in \mathcal{S}_{n,p}} s_i + \sum_{\ell \in \mathcal{L}_{n,p}^{\text{in}}} f_\ell \right) - \left( \sum_{j \in \mathcal{D}_{n,p}} d_j + \sum_{\ell \in \mathcal{L}_{n,p}^{\text{out}}} f_\ell \right) + \sum_{t \in \mathcal{T}_n} \gamma_{t,p} \xi_t = 0, (n,p) \in \mathcal{N} \times \mathcal{P}, (\pi_{n,p}); \quad (3.6)$$

$$s_i = \bar{s}_i, i \in \mathcal{S} \quad (3.7)$$

$$\xi_t \leq y_t \bar{\xi}_t, t \in \mathcal{T}. \quad (3.8)$$

Given the costs and capacity limits of suppliers, consumers and service providers, the above problem is solved and the dual variable  $\pi_{n,p}$  of the product balance constraints (3.6) is obtained. This variable is key because it sets inherent values (prices) for the products at different geographical locations (acts as the market clearing prices at which all the stakeholders in the value chain exchange products to make profit). More detailed economic properties of such framework can be found in [29, 27]

We implemented the optimization models in the Julia-based algebraic modeling package JuMP [6] and solve all problems using Gurobi 9.1.0 [16]. The code is executed on a computing server that contains a 32 cores Xeon(R) CPU E5-2698 v3 @ 2.30GHz. The optimality gap for the MILPs was set to 0.01%. The problems are computationally intensive to solve (this is a difficult problem) but were solved within 24 hrs. We highlight that our optimization framework is general (can be applied to any study region), provided that the necessary data is obtained.

## 4 Techno-Economic Analysis

We now describe the data used in our TEA analysis; the data was obtained from literature reports and from engineering insight. S-Table 2 summarizes the yield factors of each technology. For example, the input of the MRF is recyclables with an input yield factor of -1. The output product is #1 plastic bottle bale with a yield factor of 0.016; this indicates that one kg of recyclables is converted into 0.016 kg of #1 plastic bottle bale at MRF.

S-Table 3 shows the experimental data on the pyrolysis yields of each type of plastic. These conversion factors facilitate the prediction of the yield of pyrolyzing plastic mixture. We assume there

S-Table 2: Summary of technology yield factors [26, 9, 14, 32].

Technology	Input Material	Input Yield Factor	Output Material(s)	Output Yield Factor
MRF	RE	-1	#1 PB	0.016
			#2 PB	0.011
			Mixed PB	0.209
PRF	#1 PB	-1	#1 PF	1
	#2 PB	-1	#2 PF	1
	Mixed PB	-1	Mixed PF	1
PY	#1 PF	-1	PO	0.826
	#2 PF	-1	PO	0.848
	Mixed PF	-1	PO	0.768
SC	PO	-1	EH	0.211
			PR	0.130
			C <sub>4</sub>	0.095
			WAX	0.200
			GS	0.176
			FO	0.058
	FG	0.131		
LDPE POL	EH	-1	LDPE	0.97
PP POL	PR	-1	PP	0.97

S-Table 3: Pyrolysis yield of individual plastics and predicted yield of plastic mixture [32]

	HDPE	LDPE	PS	PP	PET	PVC	Predicted Yield
Gas (mass%)	17.3	15.1	3.8	13.9	37.4	2.47	18.3
Oil (mass%)	82.6	84.9	92.4	86	45.5	31.7	76.8
Char (mass%)	0	0	3.9	0.17	17.1	13.8	4
HCl (mass%)	0	0	0	0	0	53	1.3
Mixture Composition (%)	0.16	0.26	0.08	0.30	0.19	0.03	

is no synergistic effect when pyrolyzing the plastic mixture. We use the following linear formula to predict the pyrolysis yield of plastic mixture in the studied region:

$$\gamma_p^* = \sum_{i \in \mathcal{I}} \gamma_i^p \cdot x_i \quad (4.9)$$

Here,  $\gamma_p^* \in \mathbb{R}_+$  denotes the yield factor of product  $p$  (e.g., pyrolysis oil) when feeding pyrolyzer with plastic mixture. Symbol  $x_i \in \mathbb{R}_+$  denotes the mass fraction of plastic  $i$  in the plastic mixture.  $\gamma_i^p \in \mathbb{R}_+$  denotes the yield factor of product  $p$  when pyrolyzing individual plastic  $i$ . Given the yield factors of all types of plastics and the composition of plastic mixture, the product distribution of pyrolyzing plastic mixture is obtained on the last column of S-Table 3. The produced pyrolysis oil comprises 50% of naphtha, 30% atmospheric gasoil (AGO) and 20% wax.

S-Table 4 summarizes the capital expenditures (CAPEX) and operating expenditures (OPEX) of technologies in the plastic upcycling infrastructure. To account for economies of scale when evaluating CAPEX of facilities, the so-called 2/3 scaling rule was used [30]:

$$\alpha^t = \bar{\alpha}^t \cdot \left( \frac{\xi^t}{\bar{\xi}^t} \right)^\beta \quad (4.10)$$

Here,  $\alpha^t \in \mathbb{R}_+$  denotes CAPEX of technology  $t$  at a scale  $\xi^t \in \mathbb{R}_+$ . Symbol  $\bar{\xi}^t \in \mathbb{R}_+$  denotes the CAPEX of such facility at base case scale  $\bar{\alpha}^t \in \mathbb{R}_+$ ,  $\beta \in \mathbb{R}_+$  denotes the scaling factor (which is assumed to be 0.6 in this work). From this analysis, it is clear that the CAPEX of steam cracking facilities dominates.

S-Table 4: CAPEX and OPEX of technologies[26, 9, 34]

Technology	Input Material	OPEX (USD/ktonne)	Scale (ktonne/yr)	CAPEX (MM-USD)
MRF	RE	16,300	506	17.6
			2530	46.3
			5060	70.3
PRF	PB	120,000	80	34.4
			400	90.3
			800	136.9
PY	PF	30,000	36	38
			365	151
			1460	348
SC	PO	112,000	995	1147
			1990	1739
			3980	2636
LDPE POL	EH	73,000	200	322
			400	489
			800	741
PP POL	PR	165,000	200	190
			400	288
			800	436

S-Table 5 summarizes transportation costs (assuming truck hauling). The transportation cost comprises a fixed distance cost and a variable distance cost:

$$\alpha_l = \bar{\alpha}_l \cdot w + \tilde{\alpha}_l \cdot l \cdot w \quad (4.11)$$

S-Table 5: Transportation cost [28, 23]

	Distance Fixed Cost (USD/tonne)	Distance Variable Cost ( USD/tonne/km)
RE, PW, PB, PF by Truck	3.01	0.07
PO by Truck	7.66	0.095

Here,  $\bar{\alpha}_l \in \mathbb{R}_+$  and  $\tilde{\alpha}_l \in \mathbb{R}_+$  are fixed and variable distance cost. The parameter  $l \in \mathbb{R}_+$  is the transportation distance (in km) and  $w \in \mathbb{R}_+$  is the weight of product transported (in tonnes). Given the longitude and latitude of the centroid of each county, we use the Haversine formula to estimate the transportation distance.

S-Table 6: Market prices for products [3, 4, 1, 2].

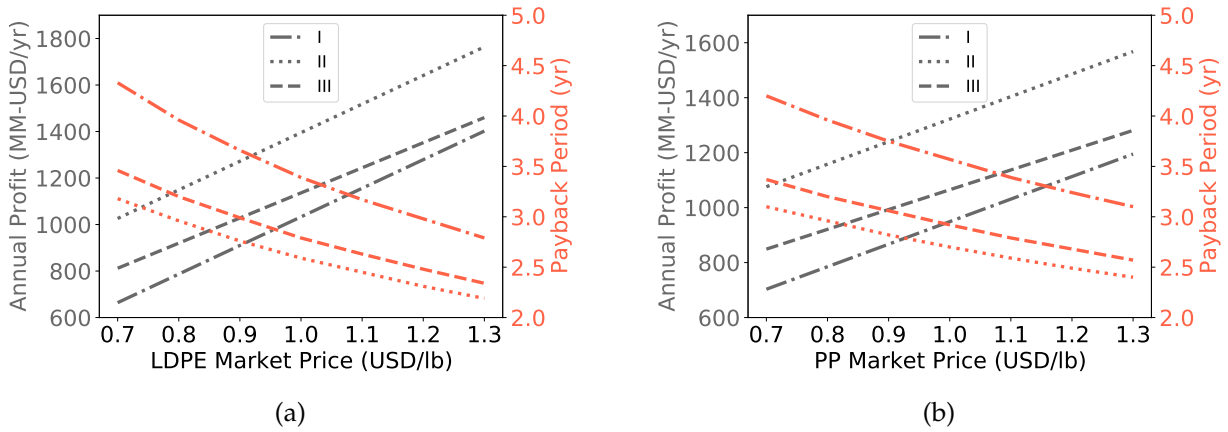
Product	Market Price	Unit
MR #1	418	USD/tonne
MR #2	991	USD/tonne
WAX	750	USD/tonne
C <sub>4</sub>	22.6	¢/lb
FG	203	¢/MMBTU
FO	492	¢/MMBTU
GS	156	¢/gallon
LDPE	1	USD/lb
PP	1.1	USD/lb
PO	500	USD/tonne

Because the sales of LDPE and PP contribute to roughly two thirds of the total revenue, the fluctuation in their prices could potentially affect the economic viability of the proposed infrastructures. A sensitivity analysis in S-Figure 9 demonstrates such impact. In this analysis, the market price of LDPE was varied by 30%. In the worst-case scenario where the LDPE price is as low as 0.7 USD per lb, the proposed infrastructures still generate more than 600 MM USD per yr of annual profit. Meanwhile, the payback periods are still less than five years. Similar trends were observed when varying the market price of PP. This analysis implies that the economic viability of proposed infrastructures is robust to the market prices of the commodities produced within the infrastructures.

## 5 Life-Cycle Analysis

As shown in S-Figure 10, the scope of this LCA study includes all processes (as well as related feeds, products, and GHG outputs) starting from the collection of waste plastics from households until the manufacturing of LDPE and PP at the polymerization process gate are accounted for. These processes include MRFs, PRFs, pyrolysis, steam cracking, and polymerization processes. In addition, the transportation steps are: recyclables transportation, plastic bale transportation, plastic flake transportation, and pyrolysis oil transportation.

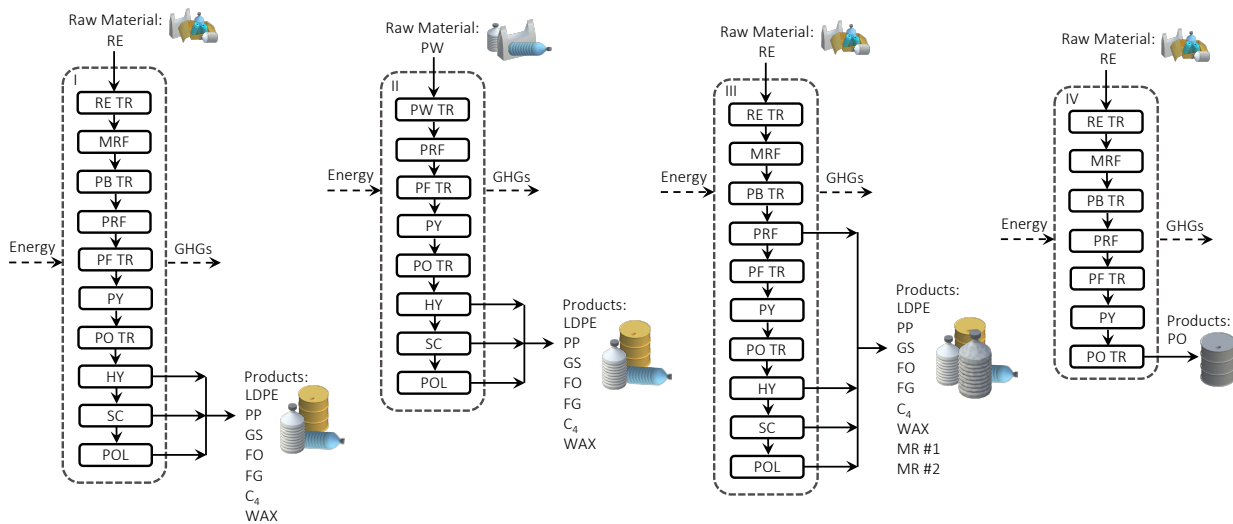
Recyclables are collected from households to an MRF. If a local MRF is not available, recyclables are collected from households to the transfer station of the county. We assume the average distance between households and the local transfer station is 20 km [13]. Transfer stations are the places where



S-Figure 9: Sensitivity analysis of (a) LDPE and (b) PP market prices and impacts on annual profit and payback period of infrastructure layouts I, II, and III.

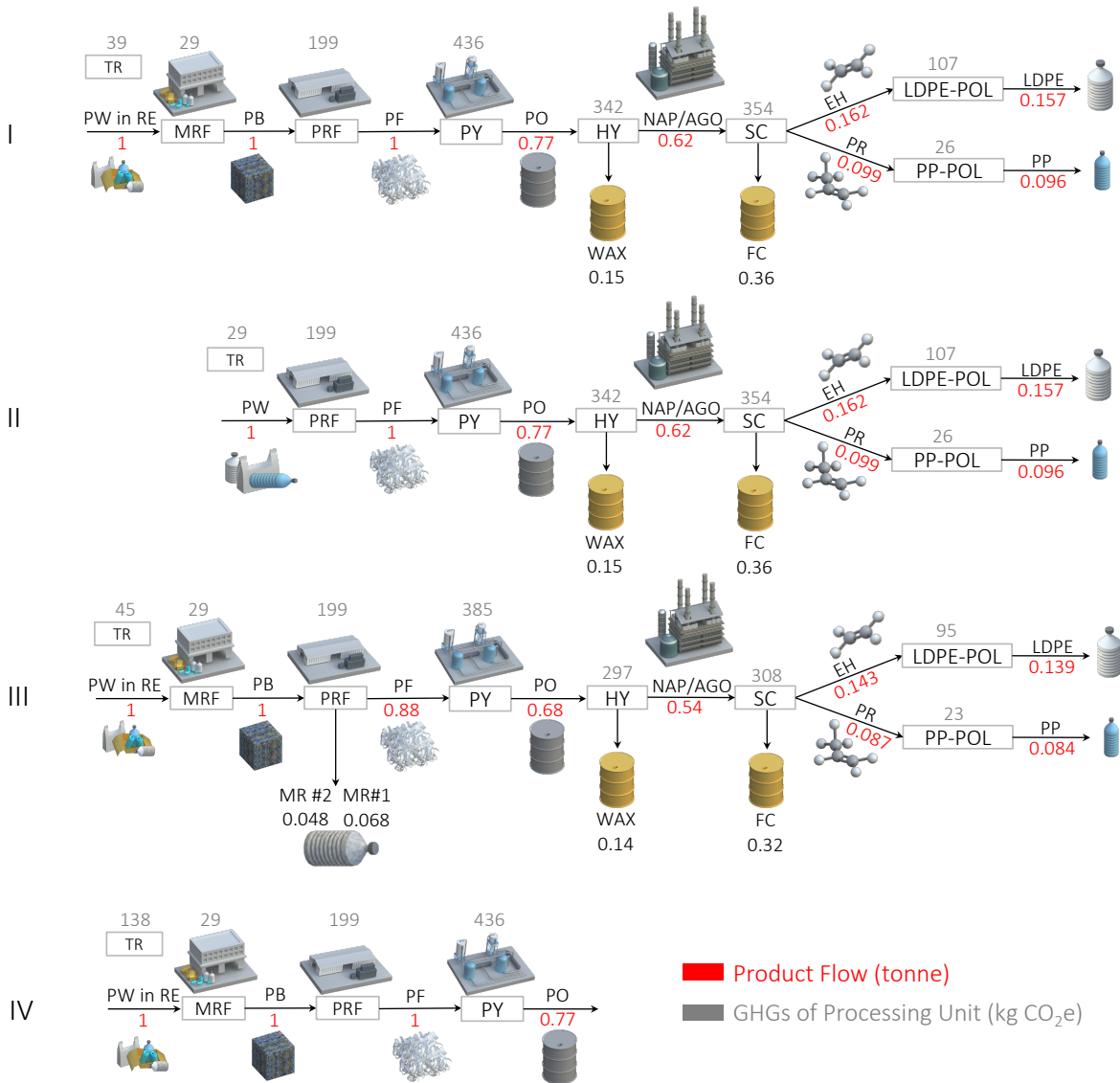
waste from local waste haulers are received. The recyclables are consolidated at transfer stations for long-distance hauling to the nearest MRFs of the neighboring counties. Therefore, recyclables transportation includes a couple of steps: collection (from households to transfer stations or to local MRFs) and long-distance transportation (from local transfer station to the nearby MRFs). In this work, the transportation tool considered is the standard 32-tonne lorry.

Global warming potential (GWP) is evaluated as the only environmental impact in this study. We quantify the global warming potential of greenhouse gas emissions with a 100-year time horizon (GWP100) using GRACI method [5]. We define the functional unit as processing one tonne of plastic waste. Table 7 presents the GHGs of processing technologies. S-Figure 11 shows the product flows and GHGs allocations.



S-Figure 10: System boundary assumed for different upcycling infrastructure layouts.





S-Figure 11: Product flows and GHGs allocations for different infrastructure layouts.

S-Table 7: Greenhouse gas (GHG) emissions of technologies [26, 31, 25, 11, 12, 10, 17].

Item	GWP 100	Unit
TR	0.0902	kg CO <sub>2</sub> -eq/tonne/km
MRF	29	kg CO <sub>2</sub> -eq/tonne of plastic
PRF	199	kg CO <sub>2</sub> -eq/tonne of plastic
PY	436	kg CO <sub>2</sub> -eq/tonne of plastic
HY	552	kg CO <sub>2</sub> -eq/tonne of oil
SC	570	kg CO <sub>2</sub> -eq/tonne of oil
LDPE POL	684	kg CO <sub>2</sub> -eq/tonne of LDPE
PP POL	273	kg CO <sub>2</sub> -eq/tonne of PP

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