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Optimal Facility Location and Sizing for Waste Upcycling Systems

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For reducing the carbon footprint of products containing polymers, recycling and upcycling of waste can make important contributions. While for certain polymers, especially for thermoplastics, melting and re-forming is attractive, although it leads to a degradation of the material properties, for others, and also after a certain degree of degradation in general, chemical processing is the most attractive option for recycling (also called upcycling). This means that from the end-of-life or production waste, valuable molecules are produced that can be fed again into the production of high-value polymers, leading to circular value chains. Such value chains can replace or reduce the use of fossil-based raw materials in polymer production, but actually realizing such value chains is a complex task. It requires setting up systemic solutions, from the collection of end-of-life or production waste over dismantling, sorting, pre-conditioning to chemical processing and downstream separation. The resulting systemic solution must be viable from an economic and from an ecologic point of view. Therefore, such systems must be analyzed and optimized from a system-wide perspective. In this work, we present a framework to model, simulate, analyze and optimize circular supply chains, and we demonstrate the potential of our framework with a case study of a value chain for the upcycling of rigid polyurethane foam waste in Germany.

1. Introduction

Chemical recycling (upcycling) of waste has become an area of particular interest over the past years with the emerging concept of circularity. Compared to mechanical recycling, chemical recycling offers the advantage of reducing the carbon footprint by not only utilizing end-of-life materials that would otherwise be incinerated or landfilled, but also producing a diverse range of virgin-equivalent valuable molecules that can replace or reduce the use of fossil-based feedstock in the production processes. Therefore, for certain types of materials such as polymers, upcycling is the most promising option to ensure that the plastic waste is recovered and reused at the highest possible value without suffering from degradation (Li et al., 2022). However, integrating chemical upcycling technologies with the waste management infrastructures is a challenging task. It requires participation of various stakeholders, development of new technologies, implementation of new regulations, and even changing the consumer behaviour. For this reason, such systems should be carefully analyzed; interactions, synergies and obstacles should be identified to ensure efficient operation and economic viability.

There is a wide variety of polymers that improve the quality of modern life, one of which is polyurethane (PU). Rigid foam polyurethanes are extensively used for insulation purposes in refrigerators and buildings due to their properties such as low weight, low thermal conductivity, insensitivity to moisture and resistance to mold (Irfan, 1998). The European Union reports a 30 % growth in the PU production in the last decade, of which 66 % is used in construction, showing that there is an increasing demand towards the material (Conversio Market & Strategy GmbH, 2018). However, the development of waste disposal and recycle infrastructures for end-of-life PU is falling short (Lardiés, 2020). Only about 2 % of the generated PU waste is mechanically recycled and the rest is incinerated (Conversio Market & Strategy GmbH, 2018).

There are only a limited number of studies that analyze the whole value chain of recycling systems based on a holistic view. Most of the studies target the electronics, automotive or paper industries. An overview is given in (Trochu et al., 2018). The main objective of our work is to build a flexible framework which supports finding an optimal design that minimizes the overall costs and environmental impact of transportation, installation and operation. For this purpose, a mixed-integer linear programming (MILP) formulation was developed to

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determine: (i) the locations and capacities of the facilities of the upcycling infrastructure and (ii) the material flows between the logistic units. The location of the waste sources as well as the amount of waste material collected are variable over time especially in the construction industry, making the process of locating different elements of the supply chain difficult. Moreover, the composition and the quality of waste is unpredictable, requiring the development of technologies that can handle different grades of waste material. All these factors make the network design problem challenging. Therefore, in this study, a scenario-based approach is adopted to investigate the robustness of the system with respect to variations in uncertain parameters. The functionality of the proposed framework is tested with a case study for Germany.

2. Model development

We pose the system-wide optimization problem as a network design problem in the form of a mixed integer linear program (MILP) in which the structure and the geographical distribution of elements of the system are optimized. An exemplary upcycling network is illustrated in Figure 1.

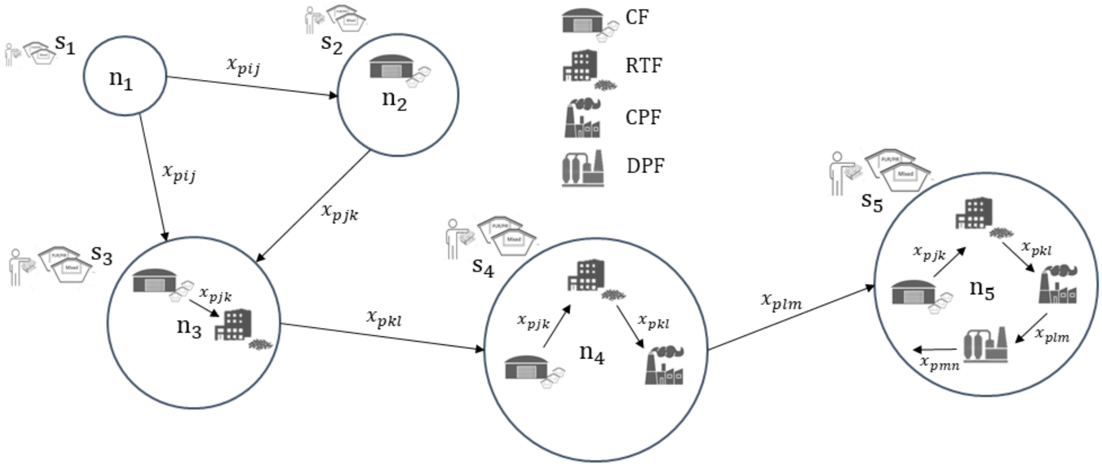


Figure 1: A schematic representation of an upcycling network (CF: Collection facility, RTF: Recovery and treatment facility, CPF: Chemical processing facility, DPF: Downstream processing facility)

2.1 Sets

In the formulation, a node represents a geographical location in the studied region. We consider each node as a waste source and as a possible location for installing facilities. In the upcycling infrastructure model, there are collection facilities (CF), recovery and treatment facilities (RTF), chemical processing facilities (CPF) and downstream processing facilities (DPF). We denote the set of sources by S. The set of materials, including intermediate and final products in the supply chain, is denoted by P. The sets of collection facilities, recovery and treatment facilities, chemical processing facilities and downstream processing facilities are denoted by CF, RTF, CPF and DPF. The set of consumers of end products (i.e. chemical production facilities) of the upgrading system is denoted by C.

2.2 Parameters

Each source $i \in S$ has a maximum waste supplying capacity $\sigma_{pi} \in \mathbb{R}^+$ for a certain material type $p \in P$. Similarly, each consumer $n \in C$ has a demand $\delta_{pn} \in \mathbb{R}^+$ for a certain product type $p \in P$. The minimum collection quota (an environmental policy parameter) for a certain material type $p \in P$ that has to be collected from the sources is η_p. The transportation cost associated with carrying one ton of material $p \in P$ per unit distance between the nodes is t_p. The transportation distances between the network nodes $j \in CF$, $k \in RTF$, $l \in CPF$ and $m \in DPF$ are represented by D_{ij}, D_{jk}, D_{kl}, D_{lm} and D_{mn}. All transportation is assumed to be carried out via roads, and the transportation distances are estimated according to the “Haversine distance” formula. Each type of facility has a maximum capacity θ_{CF}, θ_{RTF}, θ_{CPF}, θ_{DPF} $\in \mathbb{R}^+$ for allocating materials $p \in P$, an annualized installation cost α_{CF}^{I}, α_{RTF}^{I}, α_{CPF}^{I}, $\alpha_{DPF}^{I} \in \mathbb{R}^+$, an operating cost per ton of processed material α_{CF}^{O}, α_{RTF}^{O}, α_{CPF}^{O}, $\alpha_{DPF}^{O} \in \mathbb{R}^+$ and a yield factor $\gamma_{p,CF}$, $\gamma_{p,RTF}$, $\gamma_{p,CPF}$, $\gamma_{p,DPF} \in \mathbb{R}$ for certain subset of products $p \in P_{CF}^{out} \subset P$, $p \in P_{RTF}^{out} \subset P$, $p \in P_{CPF}^{out} \subset P$, $p \in P_{DPF}^{out} \subset P$ to be produced from a subset of materials $p \in P_{CF}^{in} \subset P$, $p \in P_{RTF}^{in} \subset P$, $p \in P_{CPF}^{in} \subset P$, $p \in P_{DPF}^{in} \subset P$.

2.3 Decision variables

The flows of material of a certain material type $p \in P$ between the nodes of the network are represented by a continuous variable $x \in \mathbb{R}^{+}$: Flow of material transported from $i \in S$ to $j \in CF$ is x_{pij}, similarly from $j \in CF$ to $k \in RTF$ it is x_{pjk}, from $k \in RTF$ to $l \in CPF$ it is x_{pkl}, from $l \in CPF$ to $m \in DPF$ it is x_{plm}, from $m \in DPF$ to $n \in C$ it is x_{pmn}. The installation decision of facilities is represented by a binary variable $b \in \{0,1\}$ and can be stated as follows: Installation decision of $j \in CF$ is b_j, similarly for $k \in RTF$ it is b_k, for $l \in CPF$ it is b_l, for $m \in DPF$ it is b_m.

2.4 Objective function

The objective is to minimize the total cost of the upcycling infrastructure. The first and second terms in Equation (1) account for the installation and operating costs of facilities, and the last term accounts for the transportation costs of round trips.

$$
\begin{gathered}
\min\left(\sum_{j\in CF}\alpha_{CF}^{I}\,b_j+\sum_{k\in RTF}\alpha_{RTF}^{I}\,b_k+\sum_{l\in CPF}\alpha_{CPF}^{I}\,b_l+\sum_{m\in DPF}\alpha_{DPF}^{I}\,b_m\right)+ \\
\left(\sum_{j\in CF}\alpha_{CF}^{O}\sum_{p\in P}\sum_{i\in S}x_{pij}+\sum_{k\in RTF}\alpha_{RTF}^{O}\sum_{p\in P}\sum_{j\in CF}x_{pjk}+\sum_{l\in CPF}\alpha_{CPF}^{O}\sum_{p\in P}\sum_{k\in RTF}x_{pkl}+\sum_{m\in DPF}\alpha_{DPF}^{O}\sum_{p\in P}\sum_{l\in CPF}x_{plm}\right)+ \\
2\times\left(\begin{array}{c}\displaystyle\sum_{p\in P}\sum_{i\in S}\sum_{j\in CF}D_{ij}\,t_p\,x_{pij}+\sum_{p\in P}\sum_{j\in CF}\sum_{k\in RTF}D_{jk}\,t_p\,x_{pjk}+\sum_{p\in P}\sum_{k\in RTF}\sum_{l\in CPF}D_{kl}\,t_p\,x_{pkl}+ \\ \displaystyle\sum_{p\in P}\sum_{l\in CPF}\sum_{m\in DPF}D_{lm}\,t_p\,x_{plm}+\sum_{p\in P}\sum_{m\in DPF}\sum_{n\in C}D_{mn}\,t_p\,x_{pmn}\end{array}\right)
\end{gathered} \tag{1}
$$

2.5 Constraints

The following constraints are added to the optimal facility location and sizing problem. Demand satisfaction:

$$\sum_{m\in DPF}x_{pmn}\le\delta_{pn}\quad\forall\,p\in P,\,n\in C \tag{2}$$

Minimum collection quota:

$$\sum_{i\in S}\sum_{j\in CF}x_{pij}\ge\eta_p\sum_{i\in S}\sigma_{pi}\quad\forall\,p\in P \tag{3}$$

Flow conservation at the sources:

$$\sum_{j\,\in\,CF}x_{pij}\le\sigma_{pi}\quad\forall\,p\in P,\,i\in S \tag{4}$$

Flow conservation at the facilities:

$$\gamma_{p,CF}\sum_{p\in P_{CF}^{in}}\sum_{i\in S}x_{pij}=\sum_{k\in RTF}x_{pjk}\quad\forall\,p\in P_{CF}^{out},\,j\in CF \tag{5}$$

$$\gamma_{p,RTF}\sum_{p\in P_{RTF}^{in}}\sum_{j\in CF}x_{pjk}=\sum_{l\in CPF}x_{pkl}\quad\forall\,p\in P_{RTF}^{out},\,k\in RTF \tag{6}$$

$$\gamma_{p,CPF}\sum_{p\in P_{CPF}^{in}}\sum_{k\in RTF}x_{pkl}=\sum_{m\in DPF}x_{plm}\quad\forall\,p\in P_{CPF}^{out},\,l\in CPF \tag{7}$$

$$\gamma_{p,DPF}\sum_{p\in P_{DPF}^{in}}\sum_{l\in CPF}x_{plm}=\sum_{n\in C}x_{pmn}\quad\forall\,p\in P_{DPF}^{out},\,m\in DPF \tag{8}$$

Maximum treatment capacity at the facilities:

$$\sum_{p\in P}\sum_{i\in S}x_{pij}\le\theta_{CF}\,b_j\quad\forall\,j\in CF \tag{9}$$

$$\sum_{p\in P}\sum_{j\in CF}x_{pjk}\le\theta_{RTF}\,b_k\quad\forall\,k\in RTF \tag{10}$$

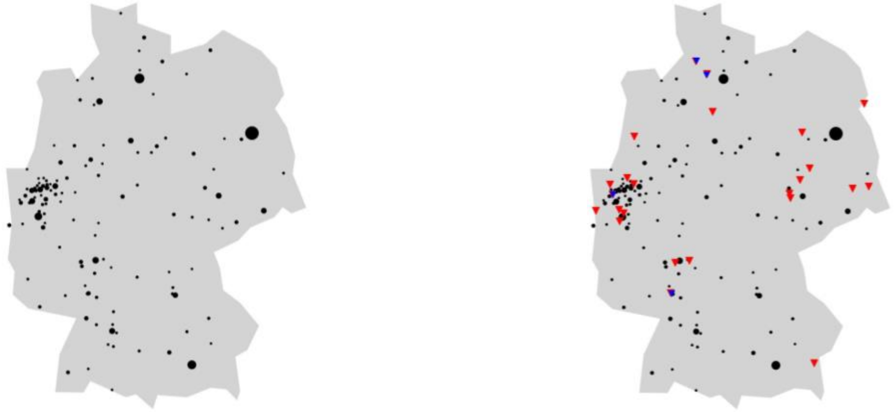
$$\sum_{p\in P}\sum_{k\in RTF}x_{pkl}\le\theta_{CPF}\,b_l\quad\forall\,l\in CPF \tag{11}$$

$$\sum_{p\in P}\sum_{l\in CPF}x_{plm}\le\theta_{DPF}\,b_m\quad\forall\,m\in DPF \tag{12}$$

The demand satisfaction constraint in Equation (2) imposes the compliance with the capacities of the consumers. The constraints given in Equations (3) and (4) ensure that the waste material is collected from the sources and shipped to collection facilities by respecting the minimum collection quota. Equations (5)-(8) enforce flow conservation at the facilities so that all the material entering a facility is processed and shipped to the next stage in the supply chain according to the yield factors associated with each technology. The maximum treatment capacities at the facilities given in Equation (9)-(12) limit the total amount of material that can be delivered to a facility.

3. Case study description and assumptions

Germany accounts for 20% of the total PU waste generated in Europe, having the largest share among European countries (Lindner, Schmitt, & Hein, 2020). About 25 % of this is coming from the construction industry. However, due to poor documentation and lack of specific data on types of PU used, waste volumes for rigid foam PU can only be estimated. The annual PU waste generation from construction materials, insulation boards and sandwich panels is assumed to be around 0.6 kg per-capita. For the purpose of this study, 123 cities in Germany with a population of over 70,000 inhabitants are chosen to be source locations and all of the German PU waste is assumed to be generated at the centroids of these cities. The amount of PU waste is calculated by multiplying the per-capita estimate by the population of the selected locations and by the whole population divided by the population of these 123 cities. The assumed PU waste distribution is given in Figure 2a.



a. b.

Figure 2: a. Polyurethane waste distribution in Germany. The relative amount of waste material is indicated by the sizes of the dots. b. Locations of existing chemical parks (red) and phosgenation plants (blue).

All 123 cities shown in Figure 2a are potential locations for opening up CFs as well as RTFs. In the case of CPFs and DPFs, 24 existing chemical parks in Germany are taken as potential locations, since these facilities require suitable infrastructures. The potential consumers who will use the produced monomers in the production of high-value polymer precursors, specifically isocyanates, are assumed to be the phosgenation plants in Germany (De Souza et al., 2021). The potential locations for opening up CPFs and DPFs along with the consumer locations are shown in Figure 2b.

The range of operations of the facilities and their yields as well as the details about the chemical processes are not yet known precisely and still under research, so we assumed plausible values that reflect the present state of knowledge. In the current study, two cases are simulated with respect to how the waste material is handled: In the first scenario (SC 1), all the construction waste is collected in mixed-waste containers and brought to CFs via skip trucks where pre-sorting takes place. The PU containing material is separated from the rest of the construction waste and transported by trucks to RTFs for mechanical separation and compression into briquettes. After this stage, the briquettes are sent to CPFs where they are pre-conditioned and converted into pyrolysis oil via a catalytic pyrolysis process (Vollmer et al., 2020). Then the pyrolysis oil is brought to DPFs for separation and purification to the desired final products. In SC 2, the PU containing waste is collected separately in big bags on-site, and not mixed with other construction waste. In this case, we assume the same transportation and size-related cost of the CFs as in SC 1 because the construction waste has to be transported and processed in any case, but the additional cost present in SC 1 for the separation of the PU containing waste from mixed waste is excluded. In SC 3 and SC 4, the influence of enforcing a more distributed structure on the overall cost is investigated by reducing the maximum capacities of CFs (SC 3) or CPFs (SC 4) to 25%; all the other parameters are same as for SC 2. A collection quota of 80 % is imposed in all scenarios. The model has 203,586 variables (294 binary, 203,292 continuous) and 2,826 constraints. It is solved in around 18 minutes.

4. Results

When the spatial distribution of the facilities is examined, it can be seen that there is a general trend irrespective of the scenario. There are multiple CFs and RTFs according to the distribution of the population that are positioned mostly at same locations to reduce transportation costs. This decentralized pattern of CFs and RTFs results from the need to minimize the transportation cost of the lightweight material. On the other hand, without capacity restrictions on the chemical processing, in the optimal structure there is a single CPF and a DPF which are placed at the same location. The centralization of the chemical and downstream processing facilities originates from the fact that these facilities are capital intensive and the capital costs are reduced by installing few large facilities. Ma et al. (2023) obtained similar results in their study in which they investigated the reverse supply chain design for post-consumer plastic waste in the US. The resulting optimal infrastructure designs of the selected scenarios are shown in Figure 3.

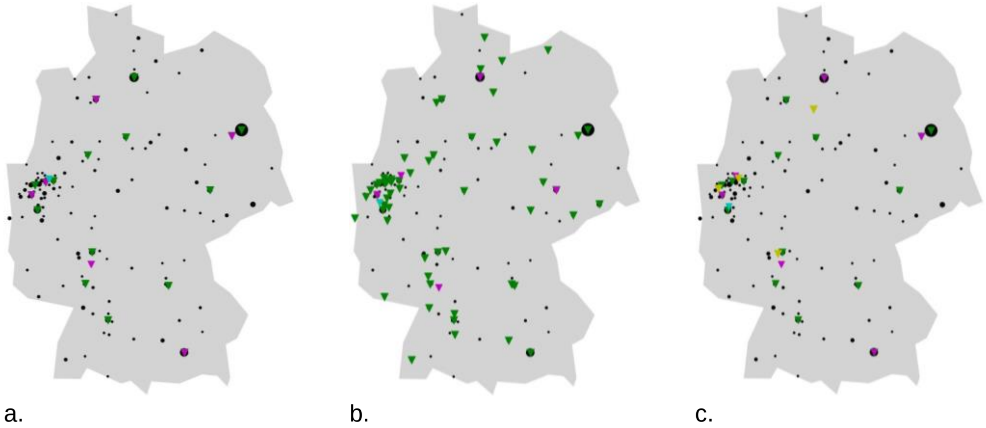


Figure 3: Optimal layouts for a. SC 2, b. SC 3 and c. SC 4, (CF: Green, RTF: Purple, CPF: Yellow, DPF: Blue)

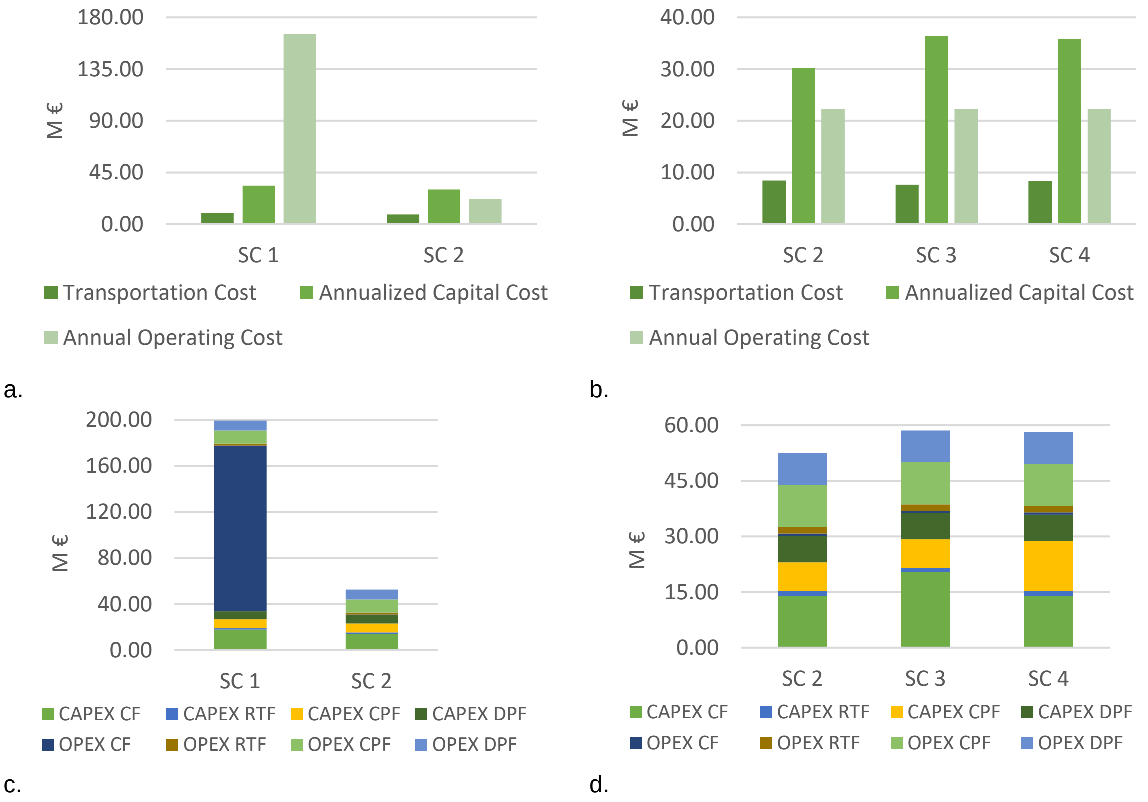


Figure 4: Total cost breakdowns of a. SC 1 and SC 2, b. SC 2, SC 3 and SC 4, Annualized capital and operating cost breakdowns of c. SC 1 and SC 2, d. SC 2, SC 3 and SC 4

In Figure 4, cost breakdowns associated with each scenario are given. Comparing SC 1 with SC 2, it can be seen that the total cost is reduced more than 3-fold by the initial collection of PU waste in big bags rather than mixed containers. The reason for this is the capital and operating expenditures of the collection facilities due to the required additional workforce and machinery to process the mixed waste. This illustrates the economic impact of implementing regulations that can substantially improve the overall operation. The trade-off between the transportation and capital costs is visible in Figure 4b. In SC 3 and 4, the capacity limit forces to open more CFs resp. CPFs, which reduces the transportation cost while increasing the capital cost. However, the total costs are still close to each other, indicating the need for more detailed investigations and taking into account other factors as e.g. getting the necessary permits and socio-political factors.

5. Conclusions

It is crucial for a more sustainable future to establish economically and environmentally viable waste handling and recycling infrastructures. From a sustainability point of view, keeping molecules intact and re-using them in chemical production processes is preferable. We therefore studied the design of a waste recycling system for rigid PU foam as a representative of high-value plastic waste. The proposed framework can be used broadly to solve large-scale facility placement and sizing problems and can provide the basis for analyzing the effect of uncertain parameters in complex large-scale problems. For example, comparative analysis on different infrastructure layouts revealed the complex trade-offs between the different costs (investment vs. transportation). Moreover, the results show that significant reductions in cost can be achieved by regulating the initial collection process. In order to guarantee a sustainable operation and to ensure compliance with the (future) regulatory framework, more sophisticated models should be developed that can also capture the dynamic nature of the upcome of construction waste, using stochastic optimization models. Lastly, we would also like to analyze the effect of environmental policies on circular value chains in more detail.

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