Design of the Systemic Modelling and Analysis Framework
D7.1

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Technical References

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Executive Summary

The CIRCULAR FOAM project aims to create a circular economy for end-of-life rigid polyurethane foams in which the recycled polyurethane (PU) is used as an input with the aim of replacing (or minimizing the use of) the virgin fossil-based raw materials in the production processes. To ensure both economic and environmental feasibility, systems, as well as products, must be designed to ensure maximum efficiency. However, integrating chemical upcycling technologies into waste management infrastructures is a challenging task since it requires interaction of various stakeholders as well as installation of specialized technologies. Therefore, such circular value chains should be carefully analyzed with respect to all degrees of freedom to reveal their true potential. In this report, design of the Systemic Modelling and Analysis Framework and first results are presented. Two different modelling platforms are created: 1. Integrated Simulation Framework and 2. Holistic Optimization Framework. The former is a heterogeneous simulation environment in which different types of detailed mathematical models can be integrated to perform sequential simulation; whereas the latter is a MILP-based holistic optimization environment the goal of which is to determine the material flows, the optimal number and the placement of facilities in the polyurethane upcycling infrastructure. The potential of the Holistic Optimization Framework is demonstrated with a case study on an abstract region without any pre-existing waste management infrastructure. The demonstration reveals that the presented framework: i. can be used to solve large-scale supply chain optimization problems to develop strategic planning steps, ii. is flexible, so any region of interest can be studied by changing and/or modifying the parameters, iii. can provide the basis for analyzing the effect of uncertain parameters in complex large-scale problems through scenario-based approach. Both frameworks are flexible tools that will support the decision making mechanism during the strategic planning phase and can help assess the potential of such circular value chains.

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1 Introduction

Reverse supply chains have become an area of particular interest over the past years with the emerging concept of circularity. Compared to a linear system, a circular system uses recycled feeds as input with the aim of minimizing the use of virgin fossil-based feedstock. In circular economy, systems and products are designed to ensure that materials are recovered and reused at the highest possible value. Therefore, by adapting circular principles throughout the life cycle of a product, the carbon footprint can be greatly reduced. While the transition to a circular economy for a more sustainable future sounds good in theory, in practice it is not that easy. It requires participation of various stakeholders, development of technologies and circular value chains, and even changing the consumer behaviour. For this reason, such systems should be carefully analysed to identify interactions, synergies and obstacles .

The objective of WP7 is to model, analyse and optimise the overall system for upcycling of polyurethane containing waste, in particular cooling appliances and construction materials, into value-added chemicals with the goal of optimizing environmental and social footprint as well as cost. As mentioned before, this system involves a wide range of interdependent operations from collection, separation and sorting of the waste material to its chemical treatment and transportation. Therefore, creating such an ecosystem in which many stakeholders interact is not straightforward, and it is important to analyse the whole value-chain based on a holistic view by considering all major degrees of freedom. This system-wide view will help to find an optimal design that balances the costs of installation and operation with the benefits of waste upcycling.

For this purpose, Task 7.1 aims at creating an integrated modelling and analysis framework in which one can simulate and optimize the polyurethane upcycling infrastructure. The results obtained will then help us to understand the potential of integrating chemical upcycling technologies into waste management infrastructures and will support making decisions during the strategic planning phase. In the following chapters, the mathematical formulation behind the framework and its implementation are presented. It should be noted that this work heavily depends on the inputs from other work packages. This means that the structure of the framework and the results generated can be revised in the light of new information and findings in the future.

2 Mathematical Formulation

In this section, the developed modelling strategies are presented in detail. The modelling concepts are introduced in Section 2.1 along with the required assumptions and parameter estimations in Section 2.2. Then, the implementation of these models in the selected environment is explained in Section 2.3.

2.1 Modelling Strategy

In the scope of this deliverable, two modelling frameworks are proposed. The first we call the "Integrated Simulation Framework" and the second the "Holistic Optimization Framework". In the following subsections, the methodologies behind these frameworks will be presented.

2.1.1 Integrated Simulation Framework

The Integrated Simulation Framework is a heterogeneous simulation environment in which detailed models of the system components can be included and linked together to perform sequential simulation. The intrinsic heterogeneity of the upcycling infrastructure requires that the framework should be able to handle models in different forms and be easily extensible when needed. What we

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mean by extensibility is that the framework being designed such that the addition of new capabilities and/or functionality is possible without large efforts. Examples of different model types are:

- Large optimization problems (e.g. Reverse Logistics)
- Complex differential and algebraic equations (e.g. Downstream Processing)
- Simpler correlations (e.g. Waste Treatment)

The framework must contain all the parameters, variables, equations and procedures that are needed to represent the system. This approach enables us to include more degrees of freedom and increases the design flexibility but at the same time increases the complexity of the framework.

In the design of the framework, "class" objects are used for the purpose of flexibility and adaptability. A class is an abstract blueprint used to create objects in programming. It provides an inheritance mechanism in which the programmer can freely create methods and attributes that contain arbitrary amounts and kinds of data within. In a way, it makes it easier for the programmer to add and bundle functionalities together. After having a blueprint, one does not need to program the same thing repeatedly. Instead, a class instance is created at a run-time by the specifying inputs, i.e. giving specific values to the attributes, that can be modified further after creation. Figure 1 shows the model classes inside the Integrated Simulation Framework.

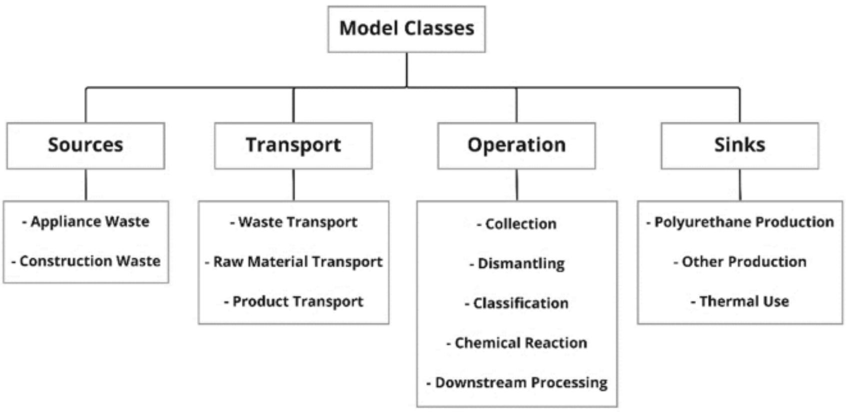

FIGURE 1. CLASSES USED INSIDE THE INTEGRATED SIMULATION FRAMEWORK

Ideally, the framework serves as a shell that encapsulates all of the subsystem models and enables easy access to variables and parameters as well as their easy manipulation. This functionality allows us to change the system parameters, including but not limited to geographical locations, waste quality and composition, capacities, product prices, process efficiencies, by only changing the parameters of the class instances and perform various simulations in order to analyze the performance and the robustness of the overall system or to generate data for other purposes. The plug-and-play approach presented here has another advantage, that is, it also enables making changes in the system configuration with minor adjustments. An exemplary instantiation of classes is shown in Figure 2.

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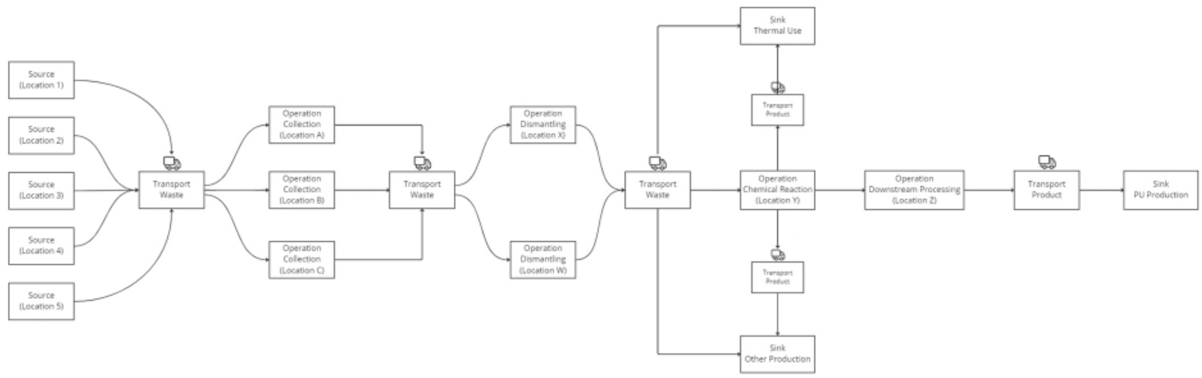

FIGURE 2. EXAMPLE INSTANTIATION OF MODEL CLASSES FOR SEQUENTIAL SIMULATION OF THE SUPPLY CHAIN

Depending on the desired system layout and the number of operations, the simulation structure, i.e. the system configuration, can easily be changed by modifying the order and the numbers of the class instances.

In this framework, there is also possibility of connecting the Aveva Process Simulator (APS) and performing simulations with detailed process flowsheets. To enable this, a module has been created using the scripting interface of APS. With this module, the user can call any existing APS flowsheet, change the variables inside the flowsheet, perform any kind of analysis, and retrieve the results.

We believe that this approach will prove to be beneficial in the later stages of the project, when more detailed process models will become available for us to exploit. For the time being, we first focus on a global analysis by adapting a bird's eye view and implementing a holistic modelling approach in the next section.

2.1.2 Holistic Optimization Framework

Inside the Holistic Optimization Framework, the network design problem is formulated as a mixed integer linear program (MILP) in which the optimal layout and economic viability of the upcycling infrastructure can be investigated.

In the formulation, a node represents a geographical location in the studied region. We consider each node as a waste source, or in other words, waste supplier, and as a possible location for installing facilities. In the current polyurethane upcycling infrastructure model, there are four types of facilities, namely, collection facilities (CF), recovery and treatment facilities (RTF), chemical processing facilities (CPF) and downstream processing facilities (DPF). We denote the set of sources with S. The set of products, including raw materials, intermediate and final products in the supply chain, is denoted with P. The sets of collection facilities, recovery and treatment facilities, chemical processing facilities and downstream processing facilities are denoted with CF, RTF, CPF and DPF, respectively. The set of consumers of end products of the upgrading system is denoted with C.

Each source $i \in S$ has a maximum waste supplying capacity $\sigma_{pi} \in \mathbb{R}^+$ for a certain product type $p \in P$. Similarly, each consumer $n \in C$ has a demand $\delta_{pn} \in \mathbb{R}^+$ for certain product type $p \in P$. The transportation cost associated with carrying one ton of product $p \in P$ per unit distance between the nodes is t_p. The transportation distances between the network nodes are represented with D_{ij}, D_{jk}, D_{kl}, D_{lm} and D_{mn}. Each type of facility has a maximum capacity θ_{CF}, θ_{RTF}, θ_{CPF}, θ_{DPF} $\in \mathbb{R}^+$ for allocating family of products $p \in P'$, an installation cost α^I_{CF}, α^I_{RTF}, α^I_{CPF}, α^I_{DPF} $\in \mathbb{R}^+$, an operating cost per ton of product α^O_{CF}, α^O_{RTF}, α^O_{CPF}, α^O_{DPF} $\in \mathbb{R}^+$ and a yield factor $\gamma_{p,CF}$, $\gamma_{p,RTF}$, $\gamma_{p,CPF}$, $\gamma_{p,DPF}$ $\in \mathbb{R}$ for certain product $p \in P$ to be produced. Each final product $p \in P$ has a certain market price denoted by $\omega_p \in \mathbb{R}^+$.

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The flow of material of a certain product type $p \in P$ between the nodes of the network is represented with variable $x \in \mathbb{R}^+$ and can be stated as follows: Flow of material transported from source $i \in S$ to collection facility $j \in CF$ is x_{pij}, flow of material transported from collection facility $j \in CF$ to recovery and treatment facility $k \in RTF$ is x_{pjk}, flow of material transported from recovery and treatment facility $k \in RTF$ to chemical processing facility $l \in CPF$ is x_{pkl}, flow of material transported from chemical processing facility $l \in CPF$ to downstream processing facility $m \in DPF$ is x_{plm}, flow of material transported from downstream processing facility $m \in DPF$ to consumer $n \in C$ is x_{pmn}. The installation decision of facilities is represented with variable $b \in \{0,1\}$ and can be stated as follows: Installation decision of collection facility $j \in CF$ is b_j, installation decision of recovery and treatment facility $k \in RTF$ is b_k, installation decision of chemical processing facility $l \in CPF$ is b_l, installation decision of downstream processing facility $m \in DPF$ is b_m.

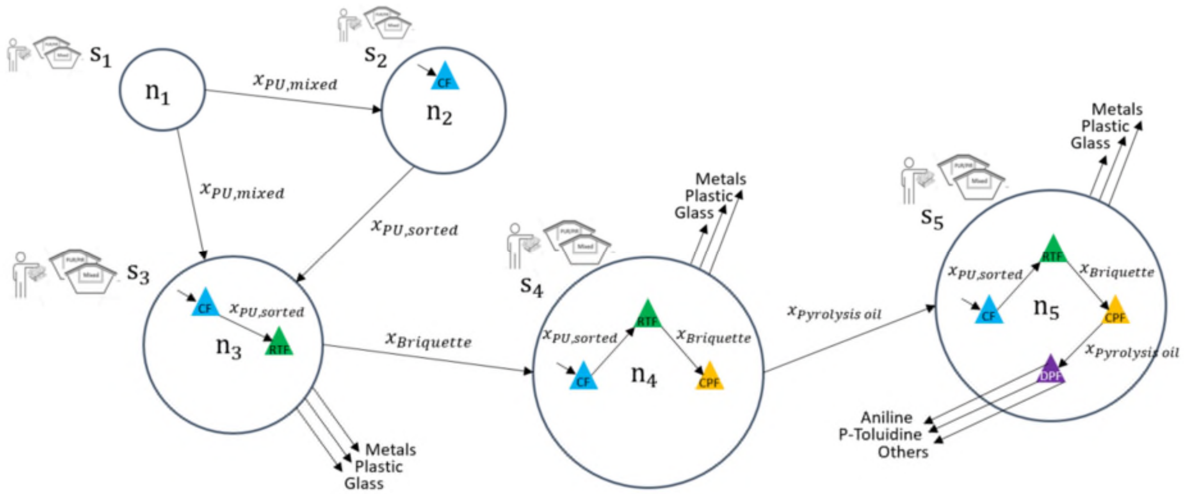

FIGURE 3. A SCHEMATIC REPRESENTATION OF THE POLYURETHANE UPCYCLING NETWORK

An exemplary structure of an upcycling network is illustrated in Figure 3. The mathematical formulation of the optimization algorithm is given below.

Objective function:

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$$
\begin{aligned}
max \sum_{p\in P} \omega_p * \sum_{n\in C} \sum_{m\in DPF} x_{pmn} \\
&- \left(\sum_{j\in CF} \alpha^I_{CF} * b_j + \sum_{k\in RTF} \alpha^I_{RTF} * b_k + \sum_{l\in CPF} \alpha^I_{CPF} * b_l + \sum_{m\in DPF} \alpha^I_{DPF} * b_m \right) \\
&- \left(\sum_{j\in CF} \alpha^O_{CF} * \sum_{p\in P} \sum_{i\in S} x_{pij} + \sum_{k\in RTF} \alpha^O_{RTF} * \sum_{p\in P} \sum_{j\in CF} x_{pjk} + \sum_{l\in CPF} \alpha^O_{CPF} \right. \\
&\left. * \sum_{p\in P} \sum_{k\in RTF} x_{pkl} + \sum_{m\in DPF} \alpha^O_{DPF} * \sum_{p\in P} \sum_{l\in CPF} x_{plm} \right) \\
&- 2 \\
&\times \left(\sum_{p\in P} \sum_{i\in S} \sum_{j\in CF} D_{ij} * t_p * x_{pij} + \sum_{p\in P} \sum_{j\in CF} \sum_{k\in RTF} D_{jk} * t_p * x_{pjk} \right. \\
&+ \sum_{p\in P} \sum_{k\in RTF} \sum_{l\in CPF} D_{kl} * t_p * x_{pkl} + \sum_{p\in P} \sum_{l\in CPF} \sum_{m\in DPF} D_{lm} * t_p * x_{plm} \\
&\left. + \sum_{p\in P} \sum_{m\in DPF} \sum_{n\in C} D_{mn} * t_p * x_{pmn} \right)
\end{aligned}
$$

Subject to constraints:

Flow conservation at sources: $\sum_{j\in CF} x_{pij} = \sigma_{pi}$ $\quad \forall\, p \in P,\ i \in S$

Flow conservation at facilities: $\gamma_{p,CF} * \sum_{i\in S} x_{pij} = \sum_{k\in RTF} x_{pjk}$ $\quad \forall\, p \in P,\ j \in CF$

$$\gamma_{p,RTF} * \sum_{p\in P'} \sum_{j\in CF} x_{pjk} = \sum_{l\in CPF} x_{pkl} \qquad \forall\, p \in P,\ k \in RTF$$

$$\gamma_{p,CPF} * \sum_{p\in P'} \sum_{k\in RTF} x_{pkl} = \sum_{m\in DPF} x_{plm} \qquad \forall\, p \in P,\ l \in CPF$$

$$\gamma_{p,DPF} * \sum_{p\in P'} \sum_{l\in CPF} x_{plm} = \sum_{n\in C} x_{pmn} \qquad \forall\, p \in P,\ m \in DPF$$

Maximum capacity at facilities: $\sum_{p\in P'} \sum_{i\in S} x_{pij} \le \theta_{CF} * b_j$ $\quad \forall\, j \in CF$

$$\sum_{p\in P'} \sum_{j\in CF} x_{pjk} \le \theta_{RTF} * b_k \qquad \forall\, k \in RTF$$

$$\sum_{p\in P'} \sum_{k\in RTF} x_{pkl} \le \theta_{CPF} * b_l \qquad \forall\, l \in CPF$$

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$$\sum_{p \in P'} \sum_{l \in CPF} x_{plm} \leq \theta_{DPF} * b_m \qquad \forall\, m \in DPF$$

Demand satisfaction:

$$\sum_{m \in DPF} x_{pmn} \leq \delta_{pn} \qquad \forall\, p \in P,\ n \in C$$

The objective is to maximize the total profit of the polyurethane upcycling infrastructure. The first term in the above equation stands for the revenue generated by selling final products, the second and third terms account for the installation and operating costs of facilities, respectively, and the last term accounts for the transportation costs for the outgoing and return trips. The flow conservation equations at the sources ensure that all of the waste material is collected and shipped to collection facilities. The flow conservation equations at the facilities guarantee that all the material entering a facility is shipped to the next point in the supply-chain while respecting the yield factors associated with each technology. The maximum capacity at the facilities limits the total amount of material that can be brought to a facility, making sure that the maximum capacity of a facility is not exceeded. The demand satisfaction constraint imposes the compliance with the requests of the consumers.

2.2 Assumptions and Parameter Estimations

This section describes the assumptions and the methodology used to estimate the necessary parameters for techno-economic analysis. Although one specific country, Germany was considered as the basis for parameter estimates, the framework is flexible, so any region of interest, including e.g. the complete European Union, can be studied by changing and/or modifying the parameters.

2.2.1 Polyurethane Waste Quantities

The annual polyurethane waste quantities are calculated using the data supplied by the partners (Interzero and Fraunhofer IML) in Work Package (WP) 3. The data suggests that, in 2021, the total number of collected “Category 1 – Heat Exchanger” waste items was 154.364 tons (Register, 2021). Moreover, ALBA Electronics Recycling stated that, within the items collected under Category 1, 90% is refrigerators. This means that, in 2021, 138.928 tons of refrigerators were collected in Germany. This information can be used in two ways: We can estimate 1) the total expected amount of polyurethane (PU) waste to be 16.671 tons (16.7 kt per annum) by assuming the PU content of a refrigerator as 12 wt.% and 2) the per-capita PU waste production to be 0,2 kg by dividing this number by the population of Germany in 2021, which was 83,2 million (Destatis, 2023). We can then use this information for generating PU waste distribution data for a region, multiplying the per-capita estimate by the population density distribution of the selected region. Similarly, according to the calculations of WP 3, PU waste generated from insulation boards and sandwich panels in 2021 was 25 kt for each type, adding up to 50 kt per annum construction waste in total for Germany. Similarly, per-capita PU waste production from construction material can be calculated as 0,6 kg. Looking at these numbers, we assume that the ratio of PU waste coming from refrigerators to construction waste is 1:3 and does not vary throughout the region under consideration, rather it is identical to the national average stated above.

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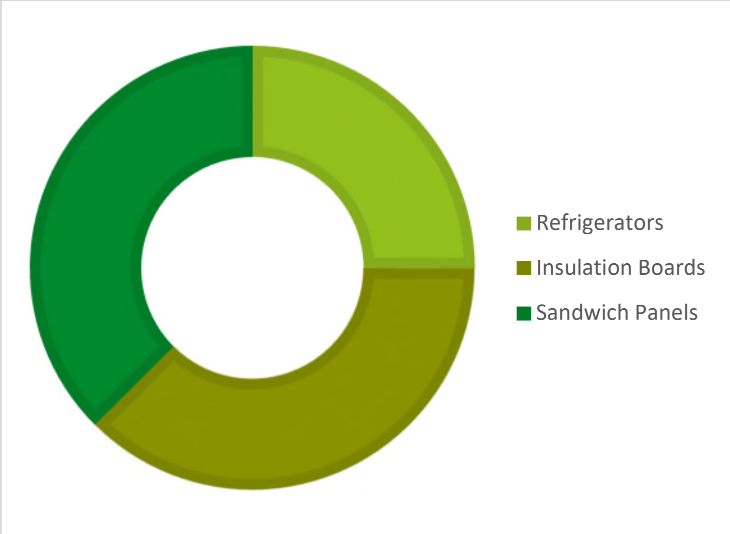

Figure 4. Nationwide Polyurethane waste composition

In the light of the data above, the input parameters regarding polyurethane volumes are as follows:

Table 1. yearly and daily Polyurethane waste amounts

	kt per year	ton per day
Appliances	16,7	46,4
Construction	50	138,9
Total	66,7	185,3

From Table 1, we can see that daily 185,3 tons of polyurethane waste are generated in Germany. We rounded up this number to 190 and used this value as the available amount of PU waste for collection (with the ratio Appliance:Construction being 1:3).

2.2.2 Transportation Costs

Transportation costs are a crucial element of any supply chain optimization problem. We used "Generalized Transport Cost" (GTC) concept in the estimation of transportation costs for each type of material transported (i.e. polyurethane, briquettes, pyrolysis oil, aniline and toluidine) (Persyn, et al., 2019).

$$Generalized\ Transport\ Cost\ =\ Distance\ Related\ Costs\ +\ Time\ Related\ Costs$$

In the above equation, distance related costs are influenced by fuel prices, fuel consumption of the vehicle, tolls, taxes and maintenance costs, whereas time-related costs are influenced by factors like travel time, average cruise speed, road characteristics, driver salaries, regulations on resting times. We decomposed two components of the GTC as:

$$Distance\ Related\ Costs = (fuel\ cost + toll) \times distance$$

$$Distance\ Related\ Costs = ([fuel\ price \times fuel\ consumption] + toll) \times distance$$

Here, tire and maintenance costs are negligible compared to the remaining elements, and neglected for simplicity. The fuel cost per km differs across EU Member States because of the differences in fuel prices. Also, fuel consumption will be affected by road properties such as slope. Both are assumed

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constant. Moreover, differences in toll costs are neglected and tax-related costs are not included in the above calculation.

$$Time\ Related\ Costs = (labor + vehicle\ cost) \times driving\ time$$

$$Time\ Related\ Costs = \left(\left[\frac{annual\ wage}{annual\ driving\ hours}\right] + \left[\frac{vehicle\ price}{useful\ life}\right]\right) \times \frac{distance}{average\ speed}$$

In time related costs, insurance and indirect costs are neglected. Here, the main component is the labor cost of the driver. In line with the regulations, assumptions are made regarding driving hours: 90 hours can be driven in 2 weeks of time, and two weeks of rest per year in addition to these compulsory resting times. This gives of 2070 hours driven per year. By dividing the annual driver wage by this estimate of hours driven per year, labor cost per hour driven is calculated, including resting times, and by dividing the vehicle price by useful life in hours, vehicle cost per hour driven is calculated. Useful life is converted into hours as follows: 15 years x (360 days / year) x (90 hours / 14 days). Here, since drivers are working with shifts it is assumed that other drivers can operate trucks. Otherwise, alternative way to calculate useful life is 2070 x 15 but either way the difference is minimal.

All transportation is assumed to be carried out via roads. The transportation distances are estimated according to the "Euclidian distance" formula and distance matrix is calculated by a custom function that takes point coordinates as inputs. Given N number of points and their coordinates (longitudes and latitudes for real geographical locations) N-by-N distance matrix is calculated automatically, corresponding to the transportation distance between each pair of points.

Lastly, transportation cost per unit distance per unit mass of material transported can be computed by dividing the above formulations by the maximum vehicle load. However, for lightweight materials such as polyurethane, the volume of the truck will be the limiting factor, rather than the load. Therefore, instead of dividing by maximum load, it should be divided by (volume of the vehicle x density of the transported material). The parameter values are given in Tables 2 and 3 (Aldrich, 2023).

TABLE 2. TRANSPORTATION COST PARAMETERS

Fuel price (€ per liter)	1,79
Fuel consumption (liter per km)	0,40
Toll cost (€ per km)	0,198
Driver wage (€ per year)	45.500
Driver hours (hours per year)	2070
Useful life (years)	15
Average speed (km per hour)	60
Density of PU (ton/m^3)	0,045
Density of briquettes (ton/m^3)	0,60
Density of pyrolysis oil (ton/m^3)	0,80
Density of aniline (ton/m^3)	1,02
Density of toluidine (ton/m^3)	0,973

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It is assumed that roll-off trucks with small containers are used for collection, bigger ones are used for transporting collected PU to waste recovery and treatment facilities and also for transporting briquettes to chemical processing facilities. In order to transport pyrolysis oil, equipment that is more sophisticated is required since pyrolysis oil is classified as corrosive. Thus, stainless steel tankers are chosen at this stage. Lastly, the final products are also transported in stainless steel tankers.

TABLE 3. TRANSPORT VEHICLE PARAMETERS

Vehicle type	Small Roll-off	Big Roll-off	Tanker
Vehicle price (€)	10.000	30.000	50.000
Max load (ton)	6	20	-
Max volume (m^3)	33	99	30-45

2.2.3 Yield Factors

In our infrastructure model, we assumed that four types of facilities (CF, RTF, CPF, DPF), each having different technologies, exist. The overall upcycling process is not yet known precisely, the range of operations at facilities and the details about the chemical processes are either not determined, or still under research. For example, collection facilities can accommodate operations such as pre-sorting, pre-treatment, shredding etc. or be only used as storage-like units where consumers bring PU waste. Therefore, for now, we investigated only one type of layout. In this layout, PU waste is collected from sources and brought to collection facilities, and then shipped to recovery and treatment facilities where it is separated and compressed into briquettes. At this step, other valuable materials such as glass, plastics and metals like iron and aluminium are recovered in reality. However, they are not considered as a revenue source in the current layout since the details about the dismantling processes (such as yield factors) are not known yet. After this stage, briquettes are sent to chemical processing facilities in which they are converted into pyrolysis oil. Then, pyrolysis oil is brought to downstream processing facilities for separation and purification to desired final products, i.e. aniline and toluidine. The set of products in this reverse supply chain layout therefore consist of polyurethane from appliances, polyurethane from construction, briquettes, pyrolysis oil, aniline and toluidine. The summary of flows is shown in Figure 5.

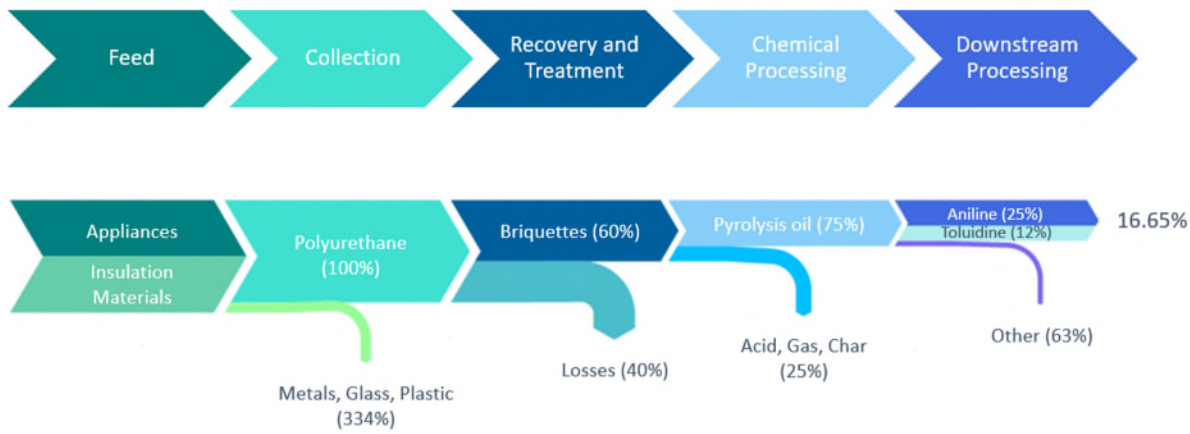

FIGURE 5. SANKEY DIAGRAM SUMMARIZING MATERIAL FLOWS IN THE INFRASTRUCTURE LAYOUT

Each facility has a yield factor relating the input flows to the output flows (e.g. how much pyrolysis oil can be produced from briquettes that are fed into the system). 5% of the collected material is assumed

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to be lost in the collection facilities during loading and unloading operations. In order to estimate a yield factor for the recovery and treatment facilities, we contacted the project partners in WP 3. The data received from Interzero is as follows:

- Processing rate of the dismantling line: 70 fridges/h
- Polyurethane recovered per fridge: 5,8 kg
- Operating with two eight-hour shifts.

In addition, we assumed the average weight of a fridge as 85 kg with 12 wt.% PU content. This gives 10,2 kg PU per fridge. According to the data above, 1120 fridges are processed per day, theoretically yielding 11,4 ton PU per day. What is recovered in reality is 6,5 ton PU per day, giving a yield factor of 0,60. This yield factor holds for an appliance dismantling process, however, since there is no technology for the construction waste at the moment, this value is used for both input streams. Lastly, since the PU pyrolysis technology is still under development, the yield factor for pyrolysis oil is taken from literature (Brown, et al., 2012) (Wright, et al., 2010), and was also discussed with the partners in WP 4. Similarly, the aniline and toluidine yields are taken from the conceptual design flowsheets developed by ETH Zurich. Table 4 summarizes yield factors associated with processes in each facility.

TABLE 4. YIELD FACTORS OF FACILITIES WITH RESPECT TO PRODUCTS

	Appliance	Construction	Briquettes	Pyrolysis oil	Aniline	Toluidine
$\gamma_{p,CF}$	0,95	0,95	0	0	0	0
$\gamma_{p,RTF}$	0	0	0,60	0	0	0
$\gamma_{p,CPF}$	0	0	0	0,75	0	0
$\gamma_{p,DPF}$	0	0	0	0	0,25	0,12

2.2.4 Market Prices, Installation and Operating Costs

The installation and operating costs are key pieces of techno-economic data. Since the associated technologies are still under development, the values presented here are just rough estimates.

The installation (capital) costs can be divided into two main components, direct costs and indirect costs (or manufacturing and nonmanufacturing capital costs). The direct costs include purchased equipment and its installation, buildings, piping, instrumentation and controls, land etc. whereas indirect costs include engineering and supervision, construction expenses, legal expenses, contractor's fee and contingencies, which are not directly related to the process operation itself. Similarly, operating costs can be divided into three categories, variable costs, fixed costs and overhead costs. The variable costs include raw materials, catalysts, solvents and utilities (electricity, water, steam, fuel, waste disposal etc.) and can be expressed per unit product produced. The fixed costs can include taxes, capital depreciation, R&D, insurance and services like accounting. This fixed part is independent of the amount of material produced or processed. The labour costs include money spent on the personnel such as managers, engineers, operators, security etc., and it can be calculated either inside variable or fixed costs, depending on the choice, or for the specific case since it is mostly a function of the installed (or planned) capacity rather than the nominal production rate (activity level of the facility). The overhead costs are related to the expenditures required for routine facility services such as medical expenses, storage facilities, safety and protection, restaurant etc.

Since the detailed estimation of each item is not possible at this point, the method of Lang factors is used to obtain an order-of-magnitude total capital cost estimate (Peters, et al., 2003). First,

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equipment costs for each processing facility were estimated with the help of project partners and literature (Ma, et al., 2023) (Zhang & Wright, 2014) (Brown, et al., 2012) (Wright, et al., 2010). Then, the capital investment is calculated by multiplying purchased equipment cost by its associated Lang factor. Similarly, due to lack of available data such as detailed process flowsheets, material and energy balances, and fixed plant capacities, the operating costs are drawn from published information on similar processes (Ma, et al., 2023) (Zhang & Wright, 2014) (Brown, et al., 2012) (Wright, et al., 2010). In calculations, variable operating costs are assumed to be 65% of the total operating expenses (Peters, et al., 2003). Table 5 summarizes reference values of the capital (CAPEX) and variable operating (OPEX) expenditures of each facility along with the selected maximum capacities for simulation. While evaluating the CAPEX for a selected capacity, so called “six-tenths-factor rule” is used to account for economies of scale (Peters, et al., 2003).

$$\alpha^{I}_{Facility} = \alpha^{Ref}_{Facility}\left(\frac{\theta_{Facility}}{\theta^{Ref}_{Facility}}\right)^{0.6}$$

Here, $\alpha^{I}_{Facility}$ is the CAPEX of facility at a scale $\theta_{Facility} \in \mathbb{R}^{+}$ and $\alpha^{Ref}_{Facility}$ denotes the CAPEX of such facility at the reference case scale $\theta^{Ref}_{Facility} \in \mathbb{R}^{+}$.

TABLE 5. CAPEX AND OPEX OF REFERENCE FACILITIES

	Max Capacity (ton/day)	OPEX (€/ton)	Reference Capacity (ton/day)	Reference CAPEX (M €)
CF	50	15	100*	1,45
RTF	50	46	100	2,88
CPF	120	28	278*	100
DPF	100	103	278	250

*100 tons per day corresponds to 36 kt per year and similarly, 278 tons per day corresponds to 100 kt per year

In the optimization the total capital investment cost calculated by the six-tenths-factor rule for a selected capacity is annualized using the “Capital Recovery Method” by assuming an interest rate of 10% and a useful life (or loan period) of 10 years (Peters, et al., 2003).

$$Annualized\ Cost = \frac{Rate}{1-(1+Rate)^{-Useful\ Life}} \times Capital\ Cost$$

In Table 6, the assumed market prices of aniline and toluidine are given (Group, 2023) (Indexbox, 2022) (Voleba, 2023) (Molbase, 2023).

TABLE 6. MARKET PRICES OF FINAL PRODUCTS

Product	Market Price (€/ton)
Aniline	1495
p-Toluidine	2400

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2.3 Implementation

Both simulation and optimization frameworks are implemented using Python programming language, and optimization problems are solved using Python interface of the SCIP Optimization Suite, PySCIPOpt (Berlin, 2023).

Instead of using an off-the-shelf modelling software such as General Algebraic Modelling System (GAMS), we chose to use Python, an object-oriented programming language, for our purposes. The reason behind this choice is the limited scope of algebraic modelling languages. Python has a rich library of built-in functions for data manipulation, and uses more concepts and constructs, whereas frameworks like GAMS have a very small language and only offer a subset of the functionalities that a solver has to offer. Therefore, it is a good idea to be flexible and not to be confined by the functionalities of commercial software while modelling complex systems.

3 Results

In this section, the proposed MILP-based holistic optimization strategy is demonstrated using an abstract study region. The goal is to determine the optimal number and placements of facilities in the polyurethane upcycling infrastructure that maximize the profit. It should be noted that the results shown here are preliminary and heavily depend on the chosen values of the techno-economic parameters.

For this case study, we created a hypothetical 500 km by 500 km region in which the polyurethane waste distribution is inhomogeneous. As stated in Section 2.2.1, the geographical distribution of waste can be correlated with the population density and therefore, waste generation per-capita values can be used to generate geographical waste distribution data while analyzing real regions. The hypothetical region is depicted in Figure 6. The amount of waste material available for collection at the sources is indicated by the sizes of the dots.

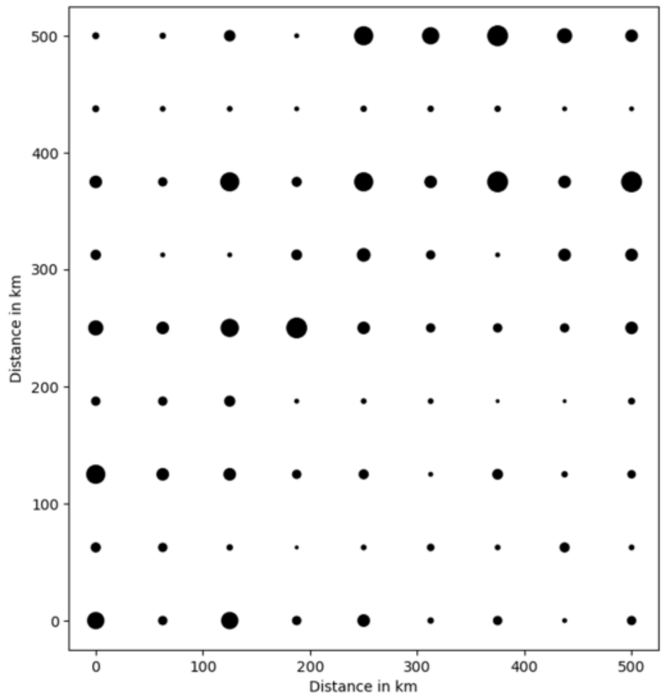

FIGURE 6. SOURCE LOCATIONS AND WASTE DISTRIBUTION IN THE HYPOTHETICAL REGION

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In this layout, there are 81 point-sources in which the waste is generated. We assume that this hypothetical region has no installed structure for collecting, treating and processing waste. As mentioned before in Section 2.1.2, all of these points are treated as possible locations for installing the facilities. The reason behind this choice is that we wanted to make the system as flexible as possible, i.e. free from all region-specific constraints such as waste collection legislations and existing facilities, and investigate the resulting infrastructure layout as a function of the parameters. However, with this choice we are confronted with increased problem complexity and computational difficulties. Obtaining exact solutions, or even high-quality approximate solutions for large-scale supply chain models (MILP-type optimization problems) is still a challenge despite the advances in computing power (Ma & Zavala, 2022). To overcome this issue in the short term, we first performed an analysis to decide on the resolution, i.e. the sufficient number of points to accurately represent the system. In Figure 7, two layouts with different number of source points are shown. The total amount of waste generated is the same in these two layouts.

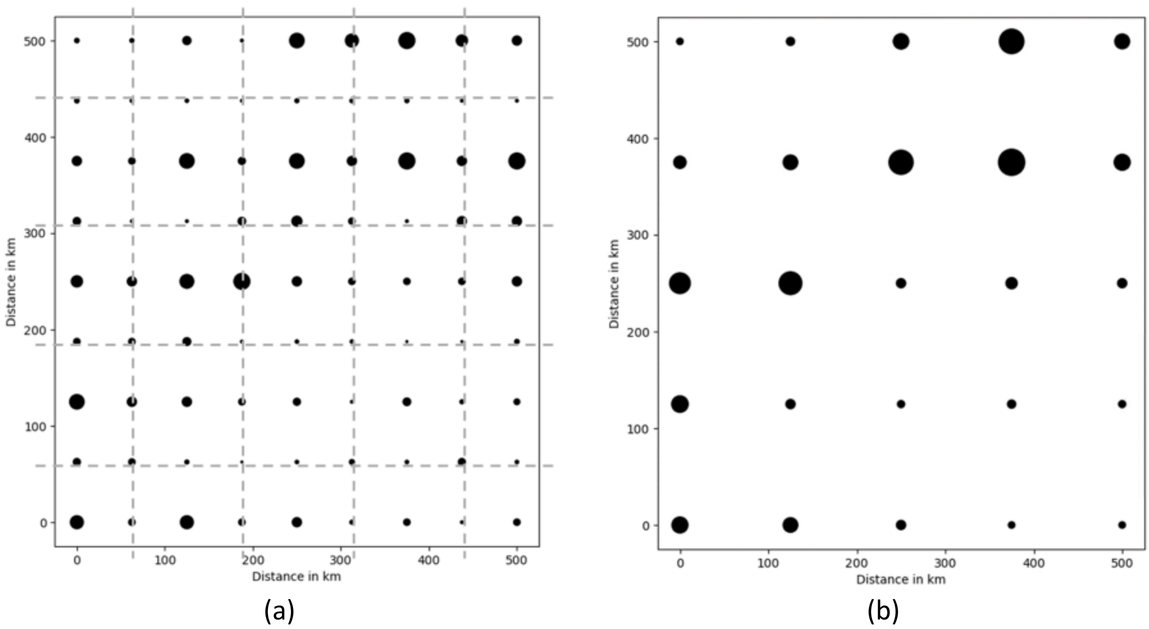

FIGURE 7. (A) HYPOTHETICAL REGION WITH 81 POINTS, (B) HYPOTHETICAL REGION WITH 25 POINTS

The resulting optimal infrastructure designs are shown in Figure 8. It can be seen that even if the locations are not identical, the difference in the objective function is only 1.4% and hence not significant. It can be concluded that using 25-point layout is sufficient for the current state of the project where the parameters are still uncertain and that the solution is not sensitive to small differences in the locations.

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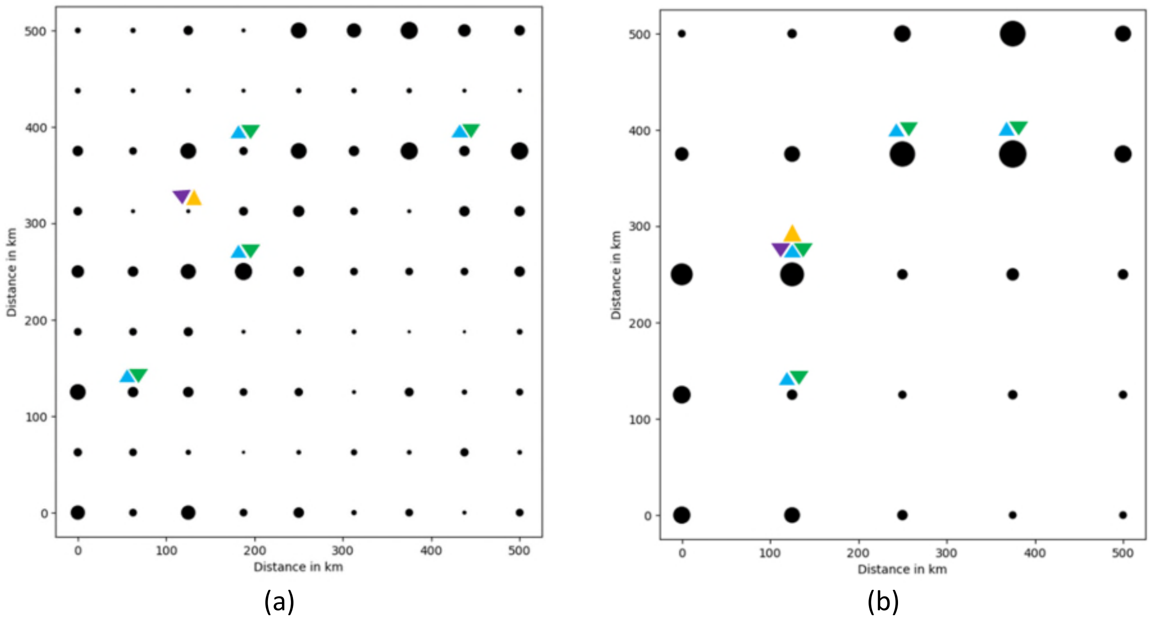

FIGURE 8. (A) OPTIMAL FACILITY LOCATIONS IN THE HYPOTHETICAL REGION WITH 81 POINTS, (B) OPTIMAL FACILITY LOCATIONS IN THE HYPOTHETICAL REGION WITH 25 POINTS (BLUE: COLLECTION FACILITIES, GREEN: RECOVERY AND TREATMENT FACILITIES, YELLOW: CHEMICAL PROCESSING FACILITIES, PURPLE: DOWNSTREAM PROCESSING FACILITIES)

Figure 9 illustrates the optimal spatial distribution of the facilities in the hypothetical region with 25 source locations. The aim was to optimally locate CFs, RTFs, CPFs and DPFs in an optimal manner maximizing profit the overall profit (or minimizing the overall losses).

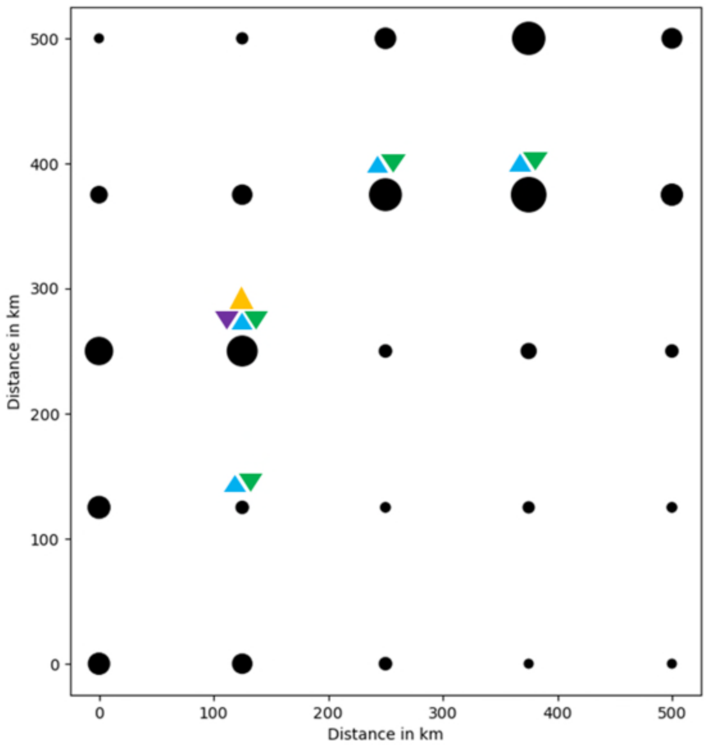

FIGURE 9. OPTIMAL DESIGN OF THE POLYURETHANE UPCYCLING INFRASTRUCTURE IN THE HYPOTHETICAL REGION WITH 25 POINTS (BLUE: COLLECTION FACILITIES, GREEN: RECOVERY AND TREATMENT FACILITIES, YELLOW: CHEMICAL PROCESSING FACILITIES, PURPLE: DOWNSTREAM PROCESSING FACILITIES)

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From the solution, it can be seen that there are multiple collection and recovery and treatment facilities placed at the same location. Putting facilities at the same location significantly reduces the transportation costs. Thus, integrating collection centers along with new/existing waste treatment centers should be considered in real regions. The placement pattern follows the waste density of the hypothetical region and it is decentralized for CFs and RTFs. This decentralized pattern indicates: 1) the need to minimize the transportation costs of the lightweight material by putting several CFs and 2) need desire to concentrate the polyurethane waste into more dense material, briquettes, by putting several RTFs by which the transportation efficiency is further increased. The centralized placement strategy of chemical and downstream processing facilities originates from the fact that these facilities are capital intensive. They usually benefit from economies of scale therefore the capital costs are reduced by installing few but large facilities.

We extended our analysis and compared the solutions of having one centralized chemical processing facility with 120 ton/day maximum capacity to having two such facilities with 60 ton/day maximum capacity. The optimal infrastructure design is shown in Figure 10. The geographical view of the layouts is almost identical, except of an additional pyrolysis plant put at the same location as collection and recovery and treatment facilities. This again eliminates transportation costs. Moreover, among the three options (locations of collection and recovery and treatment facilities) the optimal design puts the additional plant to the area where the waste density is high and to the one which is closer to downstream processing facility, as expected. When the individual elements of the cost are analysed, it is seen that an additional pyrolysis facility results in 3% decrease in overall transportation costs. On the other hand, to the effect on the overall capital cost is a 5% increase. In conclusion, when the two layouts are compared, the difference between the overall costs is 2%. Despite of the increase in the overall cost in the case of two chemical processing facilities, the values are still very close to each other. This implies that the optimal solution can change, and favour one over the other as parameters are changed/updated upon a more detailed analysis and/or if new revenue sources are added to the system.

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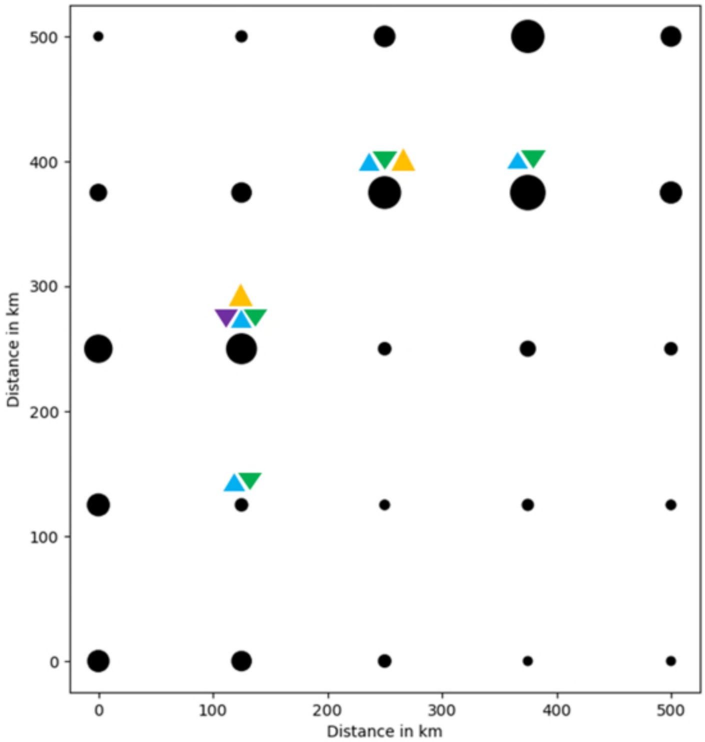
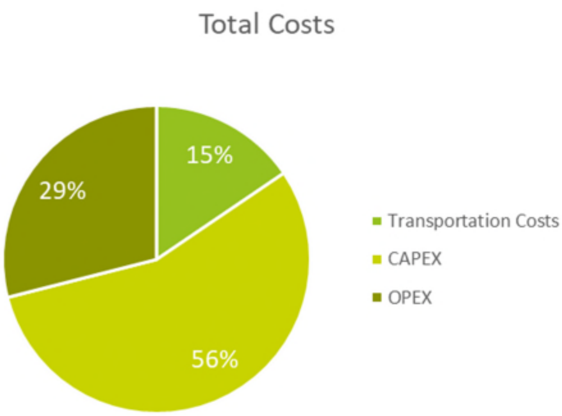


FIGURE 10. OPTIMAL DESIGN OF THE POLYURETHANE UPCYCLING INFRASTRUCTURE WITH TWO CHEMICAL PROCESSING FACILITIES (BLUE: COLLECTION FACILITIES, GREEN: RECOVERY AND TREATMENT FACILITIES, YELLOW: CHEMICAL PROCESSING FACILITIES, PURPLE: DOWNSTREAM PROCESSING FACILITIES)

In a real region, such a scenario can result if the pyrolysis plants are integrated into chemical parks. This might reduce the capital costs to some extent and make a decentralized layout more profitable. The cost breakdowns are shown in Figure11.



(a)

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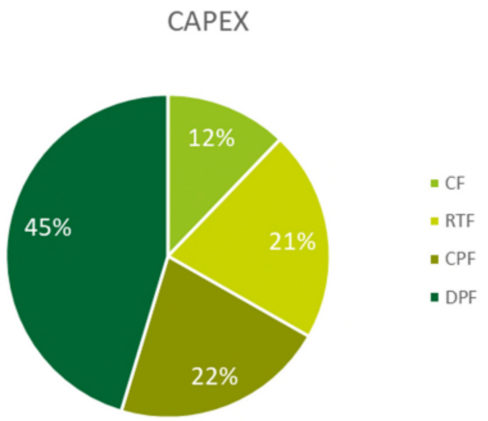
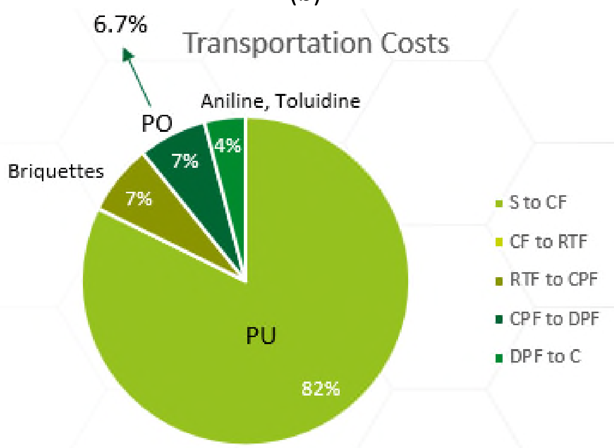


(b)



(c)

FIGURE 11. COST BREAKDOWN OF THE LAYOUT WITH TWO CHEMICAL PROCESSING FACILITIES: (A) SHARE OF INDIVIDUAL COST ELEMENTS IN TOTAL COST, (B) SHARE OF FACILITIES IN CAPITAL EXPENDITURES, (C) SHARE OF TRANSPORTING DIFFERENT MATERIALS IN TRANSPORTATION COSTS

The overall cost is dominated by installation costs, i.e. capital expenditures. As expected from the assumed capital costs, the largest share is caused by the downstream processing facility followed by chemical processing facilities (pyrolysis). When we look at the transportation costs, transporting the collected PU has the highest share since there density of the material is the lowest. In our calculations, starting from collection, we assumed that the containers contain only PU, in other words, all of the available volume of the container is occupied by polyurethane. In reality, these containers will be mixed waste. This will further decrease the transportation efficiency and increase costs significantly because each transport will yield less PU. On the other hand, transporting pyrolysis oil is still advantageous, even though it requires more expensive equipment for transport.

It is worth mentioning once again that results presented here are for a hypothetical region in which no given waste management infrastructure exists. If desired, real geographical regions with existing waste management infrastructures can also be investigated with our framework and in fact, the problem complexity will be much lower due to the fixed locations. The example was chosen to assess as well as demonstrate the functionality of the holistic optimization framework in solving a general a supply chain and facility sizing and location optimization problem. These are not final results but are simply an illustration on how such a framework can be used and extended. As we progress in the project, more analyses will be possible in order to evaluate the robustness of the system, e.g. assessing different scenarios and layouts such as integrating pre-sorting at the collection facilities, highlighting

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economic trade-offs, performing sensitivity analysis on uncertain parameters such as fuel prices, market prices, waste volumes. These analyses are important to identify and weigh the benefits of different system designs. To give an example, of all the polyurethane waste coming from insulation boards and panels, 18% is production waste, 27% is construction waste and 55% is demolition waste. This means that the highest share belongs to the stream, which is the hardest to separate, therefore increasing the transportation and processing costs. These types of trade-offs should be identified and analyzed to ensure the economic viability of the supply chain.

Lastly, the optimal designs calculated by the framework are not necessarily unique due to the nature of the solutions of mixed-integer optimization problems. This means that the same or a very similar objective value, i.e. profit or cost, can be achieved by different designs.

4 Conclusion

In this report, two modelling frameworks for the optimization and the techno-economic analysis of the polyurethane upcycling infrastructure are presented. The results of this deliverable indicate that the proposed Holistic Optimization Framework: can be used to solve large-scale supply chain optimization problems to develop strategic planning steps (such as number, location and capacity of facilities) for any geographical region and can provide the basis for analyzing the effect of uncertain parameters (e.g. annual waste generation, fuel prices, market prices, waste composition) in complex large-scale problems. As a part of our future work, we plan to extend the problem resolution and making a case study for Europe by integrating more points and real geographical locations. As a basis to solve such problems, we want to explore novel solution strategies to tackle problems of high complexity that are intractable for general state-of-the-art solvers at the moment.

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