Life cycle optimization of the supply chain for biobased chemicals with local biomass resources

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ABSTRACT

Developing a biobased chemical industry that copes with the current environmental challenges relies on understanding the influence of the different stages of the value chain on economic and environmental performance. This paper investigates the use of a life cycle optimization framework to assess trade-offs between environmental and economic criteria for designing supply chains for biobased polyethylene terephthalate as a case study. A multi-objective optimization model was formulated to account for the environmental impacts (through life cycle assessment) and total costs (through life cycle costing) of the case study. High environmental priority ($w = 0.9$) in the design of the supply chain resulted in environmental gains (in 8 out of 9 midpoint indicators) with low increments (<10 %) of the total supply chain costs. The hotspot analysis supported identifying the stages (processing plants) of the supply chain where environmental and economic improvements are required. As the environmental priority increased, a rebound effect was evidenced where the mitigation of the environmental impact in different processing plants negatively affected the economic performance of other processing plants. Therefore, close collaboration with all value chain actors is required to achieve the most optimal configuration for supply chains of biobased polyethylene terephthalate.

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1. Introduction

The global industry is one of the frontrunner sectors in developing technological solutions to the transition to a renewable carbon economy (Rissman et al., 2020). However, the industry sector was responsible for approx.—30 % of the global greenhouse gas (GHG) emissions in 2016, including emissions from energy production (Ritchie, 2020). Within the European Union (EU), the industry sector is the third-largest contributor to GHG emissions, accounting for 340 million tons of CO₂-eq in 2019 (European Environmental Agency, 2021). The mineral industry

(31 %), metal industry (23 %), and chemical industry (17 %) are currently responsible for the majority of all direct GHG emissions within the industry sector in the EU (European Environmental Agency, 2021). Despite its significant contribution to GHG emissions, the chemical industry has 'slipped under the radar' of governments searching for effective measures to reduce GHG emissions to keep global warming below 2 °C (Lim, 2021).

The chemical industry heavily relies on fossil-based resources, mainly naphtha and natural gas, for chemicals and energy production. However, the increasing awareness of the negative effect of fossil-based resources on global warming and the current high oil prices has encouraged chemical companies, private organizations, and governments to promote the use of renewable carbon (e.g., bio-based carbon) (Hong et al., 2015; IEA, 2021). Bio-based carbon is obtained from biomass (e.g., agriculture products and wood-based materials), and it has been shown to outperform fossil-based carbon in terms of GHG emissions (Garcia-Velasquez and van der Meer, 2021). Nevertheless, the intended use of biomass for biobased chemicals has raised concerns about their impact on other environmental areas, such as land use, water use, eutrophication, and biodiversity (Pawelzik et al., 2013; Weiss et al., 2012). For this purpose, the life cycle assessment (LCA) framework has been used to quantify the environmental performance

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Abbreviations: GHG, greenhouse gas; EU, European Union; LCA, life cycle assessment; OR, Operations Research; LCO, life cycle optimization; PET, polyethylene terephthalate; LCC, life cycle costing; PTA, terephthalic acid; EG, ethylene glycol; MCDA, multicriteria decision analysis; GWP, Global Warming Potential; ALOP, Agricultural Land Occupation Potential; HTP, Human Toxicity Potential; WDP, Water Depletion Potential; FEP, Freshwater Eutrophication Potential; TAPF, Terrestrial Acidification Potential; MEP, Marine Eutrophication Potential; ODP, ozone depletion potential; POFP, photochemical oxidant formation potential; FETP, freshwater ecotoxicity potential; MILP, Mixed Integer Linear Program; FDP, Fossil Depletion Potential; PMFP, Particulate Matter Formation Potential; ERP, environmental reduction potential; SCTC, supply chain total cost.

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of a product throughout its life cycle and estimate the product's environmental impact on the ecosphere using different indicators, such as global warming potential, land and water use, eutrophication potential, among others (Hauschild et al., 2017).

LCA is becoming more relevant as it is expected to play an essential role throughout the policy definition and formulation, aiming to support policy-makers (Cristobal-Garcia et al., 2016). Within the industrial sector, several organizations and researchers have raised their voices on using LCA as a core method to promote the implementation of innovative technologies: biopolymers (Carus et al., 2019; European Bioplastics e.V., 2019), paper and pulp (Gaudreault et al., 2009), and in general the scale-up of chemical processes (Maranghi et al., 2020). However, environmental indicators do not play an important role in existing decision-making practices in the industry sector, where economic indicators (typically costs or profit) have the highest priority. New initiatives such as the carbon neutral industry created a way to lead the industrial sector to reach climate neutrality while mitigating adverse environmental impacts (European Commission, 2018). Nonetheless, the scope is still limited to GHG emissions despite the increasing awareness of the industry sector.

GHG emissions have been included in the decision-making process to design supply chains since it is one of the most critical factors in the current climate breakdown (Cambero et al., 2016). However, the use of multiple environmental impacts (e.g., land use, eutrophication, acidification) in decision-making is getting more attention. These environmental impacts clearly describe the interaction between the technosphere (human-made processes) and the ecosphere (ecological systems) (Pieragostini et al., 2012). This interaction is typically referred to as the cause-effect chain. There are two schools of methods on how to model this cause-effect chain: problem-oriented and damage-oriented methods. The former (based on midpoint indicators) restricts the quantitative modeling at the early stages of the cause-effect chain (e.g., climate change, human toxicity, acidification). The latter (based on endpoint indicators) attempts to model the cause-effect chain up to the damage itself (e.g., damage to human health, damage to ecosystems, and damage to resource availability) (Bojarski et al., 2009). Most supply chain models use endpoint indicators (Mota et al., 2015; Santibañez-Aguilar et al., 2011; Singlitico et al., 2020). Contrarily, midpoint indicators are not widely included in quantitative models. (Sabio et al., 2012) presented a bi-objective optimization model for designing hydrogen supply chains in Spain using midpoint indicators as environmental criteria. The authors normalized the midpoint indicators to the same reference (normalization method) to communicate the results, describing the trends shown by the different midpoint indicators. Similarly, Ren et al. (2015) used midpoint indicators to develop a life cycle sustainability assessment for bioethanol production in China. The authors highlighted the importance of using midpoint indicators to translate stakeholders' priorities in selecting the most suitable feedstock for bioethanol production.

Different methods exist to account for environmental criteria (midpoint or endpoint indicators) within optimization models. Two of the most used methods are monetary and non-monetary valuation approaches. On the one hand, monetary valuation methods aggregate the results from the environmental criterion in one single indicator, generally in monetary terms (Arendt et al., 2020). The single indicator expresses the total environmental cost of the different solutions (Pizzol et al., 2015). The use of monetary valuation methods is straightforward and is considered helpful for decision support since it allows easy communication and interpretation by the company management and policy-makers (Amadei et al., 2021). However, determining the correct monetary value for the different environmental criteria is challenging due to uncertainties in the monetary valuation methods (Arendt et al., 2020). Most supply chain models using monetary valuation focus on one environmental criterion (mostly GHG emissions) (Chaabane et al., 2012; García-Velásquez et al., 2022c; Malladi and Sowlati, 2020).

On the other hand, the non-monetary valuation method allows the evaluation of supply chain configurations based on the preferences and priorities (not necessarily costs) set by the decision-makers (Proctor and Drechsler, 2006). This valuation method has been widely explored in the optimization of chemical value chains since (Azapagic and Clift, 1999) developed the life cycle optimization (LCO) framework to include LCA as a tool to quantify the environmental impact of the whole value chain. Decision-makers can explore different solutions that satisfy each criterion since LCO allows the inclusion of other constraints (e.g., economic, social, or operational) within the optimization model without aggregating them in the same objective function.

This paper focuses on two aspects:

- Assessing the contribution (in terms of economic performance and environmental impact) of using midpoint indicators in the strategic design of biobased supply chains, and
- Providing a detailed analysis of the trade-offs between environmental impacts (based on midpoint indicators) and supply chain costs to support decision-makers in selecting suitable solutions (supply chain configurations) where both environmental and economic criteria are fulfilled.

For this purpose, the value chain for biobased polyethylene terephthalate (PET) production using biomass crops (sugar beet and *miscanthus*) is selected as a case study. The design of the biobased PET supply chain is done following the LCO framework proposed by Azapagic and Clift (1999). The economic performance of the supply chain is measured using the life cycle costing (LCC) framework (Ciroth et al., 2008). Similarly, the environmental impact of the supply chain is calculated using the LCA framework. A hotspot analysis approach is used to determine the supply chain nodes (processing plants) with the highest contribution to the change in economic and environmental performance.

2. Methods

2.1. Problem statement

PET is one of the most used polymers worldwide for different packaging and clothing applications. Within the packaging application, PET is well known for its use in manufacturing plastic bottles for beverages. Due to the variety of bottle shapes (depending on the customer requirements), the PET bottle-grade pellets are pre-shaped into pre-form PET bottles (see Fig. 1) that can be used to produce PET bottles by each customer. This study covers the supply chain until the pre-form PET bottle is produced.

PET polymer is produced by the polycondensation of purified terephthalic acid (PTA) with ethylene glycol (EG). The production of 1 kg of bottle-grade PET contains 30 % by weight of EG and 70 % by weight of PTA. The EG production includes the conversion of sugar beet (juice) into ethanol through fermentation (Plant A). From this process, sugar beet pulp is obtained as a co-product of the biorefinery. Then, ethylene is produced by bioethanol dehydration (Plant B). Finally, ethylene is converted into ethylene oxide as an intermediate for EG production (Plant C). The PTA production involves the thermochemical conversion (fast pyrolysis) of *miscanthus* into bio-oil (Plant F) as an intermediate product for para-xylene production and, subsequently, PTA (Plant M).

Given

- The availability and costs of feedstock in the different locations;
- A set of known and potential locations of the plants;
- The capacity limitations of the plants;
- The conversion efficiency of the technology in the plants;
- Investment and operating costs (e.g., reagents costs, utility costs, labor costs) of the plants;
- Transportation distances and costs (fixed and variable) between the plants;
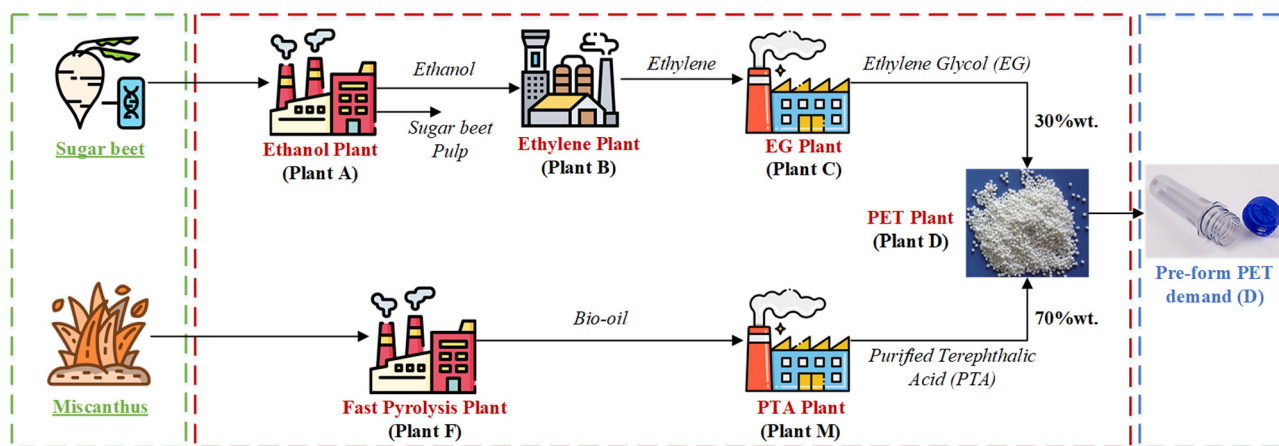
Fig. 1. Visualization of the supply network under consideration (based on the case study).

• Environmental impacts of feedstock per location and the plants;
• Environmental impacts of transportation between the plants;
• Demand location and required volume;

The model proposed in this study aims to evaluate how the increment in the environmental priority influences the supply chain configuration for biobased PET production. The objective is to minimize the total cost and the environmental impact under the constraint that the required demand is supplied to the customers (as bottle-grade PET). The decisions to be made are strategic choices, such as the location and amount of feedstock suppliers, plant locations, and flow rates between the plants.

2.2. Life cycle optimization of the biobased polyethylene terephthalate production

The LCO framework developed by Azapagic and Clift (1999) consists of four steps:

(i) LCA and LCC of the proposed case study.
(ii) A mathematical formulation of the optimization problem.
(iii) Solution of the multi-objective optimization model (economic and environmental criteria) for the design of supply chains.
(iv) Multicriteria decision analysis (MCDA) to select the best solutions.

This study aims to provide insights to decision-makers on the importance of accounting for midpoint indicators in the design of biobased PET supply chains. Therefore, this study focuses on the first three steps of the LCO framework. Section 2.2.1 elaborates on the data and procedure done to perform the LCA and LCC of the case study. Afterward, Section 2.2.2 describes the economic and environmental criteria used in the optimization problem. Finally, the solution procedure of the multi-objective optimization model is presented in Section 2.2.3.

2.2.1. Data collection for the optimization model

The first two steps of the LCO framework involve developing the LCA and LCC model. LCA allows quantifying the environmental impact of a product or system throughout its life cycle (ISO, 1997), while LCC allows estimating the business costs of a product's life cycle (production, use, end-of-life) (Ciroth et al., 2008). A cradle-to-gate approach was considered, starting from the feedstock collection through the manufacturing (plants) until the product is delivered to the customer (demand).

For this purpose, data on the economic and environmental criteria were collected from different literature sources:

• Economic and environmental data for the EG production using sugar beet as feedstock was collected from García-Velásquez et al. (2022c).
• Environmental data for the PTA production using Miscanthus was collected from Gian et al. (2022).
• Economic data for the PTA production using Miscanthus was calculated following the procedure reported in de Jong et al. (2015). The dataset is available as Zenodo repository [dataset] (García-Velásquez et al., 2022a).
• The data collected for the economic and environmental performance of the different nodes (suppliers and plants) is available as Zenodo repository [dataset] (García-Velásquez et al., 2022b).

The environmental impact assessment of the biobased PET production was performed using the ReCiPe 2016 method V1.3 (hierarchist perspective) at the midpoint level, including 17 impact categories, such as ozone depletion potential (ODP), photochemical oxidant formation potential (POFP), freshwater ecotoxicity potential (FETP), among others. The hierarchist perspective is widely used in LCA studies since scientific and political bodies back up the included facts to estimate the characterization factors in the ReCiPe method (de Bruyn et al., 2018). The list of 17 impact categories is included in the online dataset (García-Velásquez et al., 2022b). A subset of 9 environmental impact categories was selected for further analysis: Global Warming Potential (GWP), Agricultural Land Occupation Potential (ALOP), Human Toxicity Potential (HTP), Water Depletion Potential (WDP), Freshwater Eutrophication Potential (FEP), Terrestrial Acidification Potential (TAPF) and Marine Eutrophication Potential (MEP). These categories were selected based on previous publications that studied the environmental challenges of biobased materials production (Pawelzik et al., 2013); a review of the available literature (at that time) on LCA of biobased materials (Weiss et al., 2012); and the use of approaches as the Production Composition Analysis (PCA). This approach aims to determine the set of midpoint indicators that cover >90 % of the variance of the total environmental impact of different products (Steinmann et al., 2016). Additionally, Fossil Depletion Potential (FDP) and Particulate Matter Formation Potential (PMFP) were included to account for the environmental impacts of transportation between the nodes.

2.2.2. The mathematical formulation of the economic and environmental objectives

This section includes the description of the developed Mixed Integer Linear Program (MILP) for designing supply chains, including two main

objectives: minimizing the total supply chain cost and the environmental impact. This multi-objective model is an extension of the single-objective model reported in García-Velásquez et al. (2022c). The objective functions and model constraints are presented in the remainder of this section. A detailed description of the parameters and variables that are used in Eqs. (1)–(14) is presented in Appendix A.

a) *Economic objective function*

The economic objective, given in Eq. (1), aims to minimize the total supply chain cost, including the *feedstock production costs* (first term), the *capital and operating costs* (second term) of the supply chain, the *transportation costs* (third term), and *the revenues from selling co-products (sugar beet pulp) from the ethanol plant* (fourth term).

$$\min \sum_{i \in V^S} \sum_{a \in \delta^+(i)} \left(c_i^B x_a^B + c_i^M x_a^M \right) + \sum_{i \in V \setminus V^S} \left(f_i^V y_i + c_i^P x_i^P \right) \\ + \sum_{a \in A} \left(f_a^T t_a + c_a^T x_a \right) - \sum_{i \in V^A} p^{SBP} x_i^{SBP} \tag{1}$$

b) *Environmental objective function*

The LCA results are summarized in the environmental impact (E) of the individual midpoint indicators (e), defined as the potential impacts on the ecosystem, human health, and depletion of natural resources (Hauschild et al., 2017). The objective of the environmental function is to minimize the environmental impact (E) for each midpoint indicator (e) from the *transportation between nodes* (first term) and *the processes* (second term) in each plant, as represented in Eq. (2).

$$\min \quad \varepsilon_e^T \left(\sum_{a \in \delta^+(i), i \in V \setminus \{V^S \cup V^D\}} d_a x_a + \sum_{a \in \delta^+(i), i \in V^S} d_a \left(x_a^B + x_a^M \right) \right) + \sum_{i \in V \setminus V^S} \varepsilon_{ei}^P x_i^P \quad \forall e \in E \tag{2}$$

c) *Model constraints*

The multi-objective optimization model is subjected to the following constraints.

• *Supply constraints:* The amount of feedstock (sugar beet and miscanthus) to be transported to different nodes is restricted by the availability in the region.

$$\sum_{a \in \delta^+(i)} x_a^B \leq q_i^B \quad \forall i \in V^S \tag{3}$$

$$\sum_{a \in \delta^+(i)} x_a^M \leq q_i^M \quad \forall i \in V^S \tag{4}$$

• *Mass balance constraints:* Input and output mass flow rates from each supplier and plant.

$$\gamma_i \sum_{a \in \delta^-(i)} x_a^B = \sum_{a \in \delta^+(i)} x_a = x_i^P \quad \forall i \in V^A \tag{5}$$

$$\gamma_i^{SBP} \sum_{a \in \delta^-(i)} x_a^B = x_i^{SBP} \quad \forall i \in V^A \tag{6}$$

$$\gamma_i \sum_{a \in \delta^-(i)} x_a^M = \sum_{a \in \delta^+(i)} x_a = x_i^P \quad \forall i \in V^F \tag{7}$$

$$\gamma_i \left(\sum_{a \in \delta^+(j), j \in V^C} \gamma_i^C x_a + \sum_{a \in \delta^+(j), j \in V^M} \gamma_i^M x_a \right) = x_i^P \quad \forall i \in V^D \tag{8}$$

$$\gamma_i \sum_{a \in \delta^-(i)} x_a = \sum_{a \in \delta^+(i)} x_a = x_i^P \quad \forall i \in V \setminus \left(V^S \cup V^A \cup V^F \cup V^D \right) \tag{9}$$

$$\sum_{i \in V^D} x_i^P = D \tag{10}$$

• *Capacity constraints:* the mass flow rate among plants is restricted by the processing capacity of each plant.

$$x_i^P \leq Q_i y_i \quad \forall i \in V \setminus V^S \tag{11}$$

• *Linking constraints:* As soon as x_a is positive (a quantity is transported over the arc a), the corresponding t_a variable should be set to 1. This is achieved with a *big M constraint*, in which M represents a value that is a large number – sufficiently large to make sure the constraint is satisfied for every quantity x_a

$$x_a \leq M t_a \quad \forall a \in A \tag{12}$$

2.2.3. Solution of the multi-objective optimization model

The overall MILP can be expressed as shown in Eq. (13).

$$\min \begin{bmatrix} Economic\ Obj. \\ Environmental\ Obj._{\cdot e} \end{bmatrix}$$

$$subject\ to\ Eq.1 - 12 \tag{13}$$

The result of the optimization model is a set of Pareto optimal solutions (referred to as the Pareto frontier). This Pareto frontier represents the trade-off between the total supply chain costs and the environmental impact of individual midpoint indicators. Note that the environmental objective is expressed as a function of the midpoint indicators e. Pareto optimal solutions are represented by solving a set of bi-objective models to allow for structured analysis and visualization of the solutions. The supply chain costs are optimized separately against one of the selected midpoint categories in each model.

The weight sum method was used to solve each bi-objective optimization model and generate the corresponding Pareto frontier (Marler and Arora, 2010). Solving the optimization problem using the weighted sum method entails selecting scalar weights w_i and minimizing the following objective function, as shown in Eq. (14).

$$\min \quad (1 - w) * Economic\ Obj. + w * Environmental\ Obj._{\cdot e}$$

$$subject\ to\ Eq.1 - 12 \tag{14}$$

In this study, the w values refer to the decision-makers priority for the environmental criterion over the economic criterion. A w value of 0.1 means that high priority is given to the economic cost of the supply chain, while low priority is given to the environmental criterion. Contrary, a w value of 0.9 means a high priority for the environmental criterion and a low priority for the economic criterion.

3. Results

3.1. Effect of environmental prioritization on the environmental and economic performance of the biobased polyethylene terephthalate

In this study, the importance of the selected impact categories on the design of the biobased supply chain was estimated using two parameters: *environmental reduction potential (ERP)* and *supply chain total cost (SCTC)*, as shown in Eqs. (15)–(16). The ERP refers to the relation between the environmental impact of a selected midpoint indicator at any w value compared to the reference value ($w_{ref} = 0$). Similarly, SCTC refers to the relation between the total supply chain costs at any w value compared to the reference value ($w_{ref} = 0$). These parameters were selected for two reasons: first, to determine the positive or negative effect of increasing the environmental priority in the design of the biobased PET supply chain compared to the reference case, where no priority is given to the environmental criteria. Second, to compare the response of each of the selected midpoint indicators in the economic and environmental performance of the supply chain as the environmental priority increases ($w > 0$).
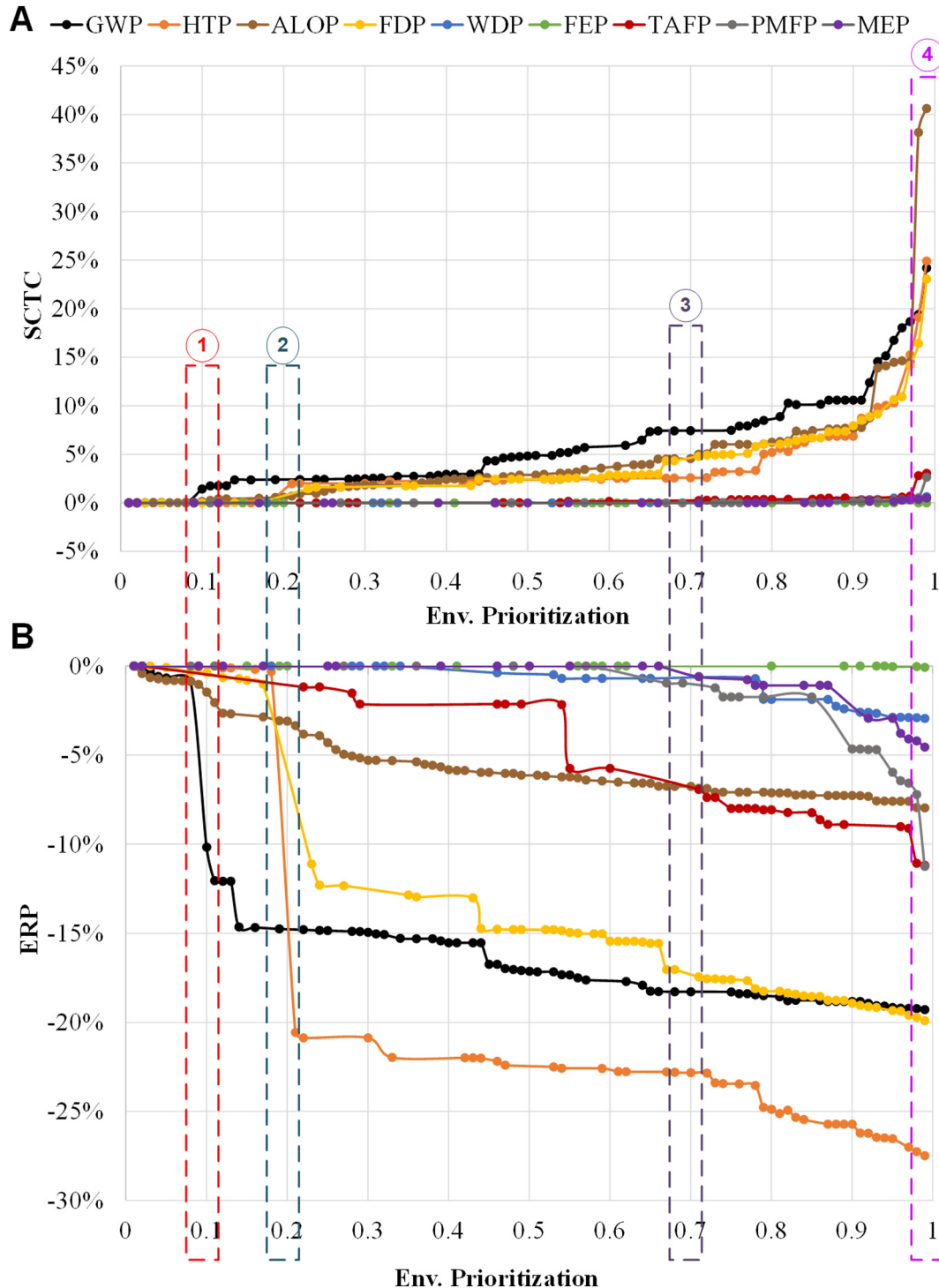

Fig. 2. Effect of environmental priority (*w* value) in the SCTC (A) and ERP (B) of selected impact categories.

$$\%ERP = \frac{E_\mathrm{w} - E_{w_{ref}}}{E_{w_{ref}}} \times 100 \qquad (15)$$

$$\%SCTC = \frac{Cost_\mathrm{w} - Cost_{w_{ref}}}{Cost_{w_{ref}}} \times 100 \qquad (16)$$

The effect of environmental prioritization (w value) on the SCTC and the ERP for the selected environmental impact categories is presented in Fig. 2. First, the supply chain costs increase, and the environmental impact is reduced when the w value increases, i.e., there is a high priority for reducing the environmental impacts compared to supply chain costs. Four w values are highlighted (see dashed squares in Fig. 2), where different trends in the ERP and SCTC of the biobased PET supply chain were noticed. At low environmental priority (dashed squares 1 and 2), the highest ERP was obtained for the midpoint indicators GWP and HTP, reducing 15 % and 21 %, respectively. Interestingly, this high reduction potential can be reached with a slight increase in the SCTC (approx. 2 %). As the environmental priority increases (dashed square 3), the reduction potential from GWP and HTP was hindered by the increase in the SCTC, i.e., an ERP of 18 % (in the case of GWP) requires an increase of 7 % in the SCTC that is more than three times the investment required at $w = 0.2$. Low supply chain costs (<5 %) were needed to increase the ERP of FDP, ALOP, and TAFP. The ERP of most midpoint indicators increased as high priority was given to the environmental criteria over the economic one (dashed square 4). However, a negative influence on the SCTC was shown for half of the midpoint indicators: ALOP, GWP, HTP, and FDP. Finally, high environmental priority provided benefits for the midpoint indicators TAFP, PMFP, MEP, and WDP since they required less than a 5 % increase in the SCTC to reach a modest ERP ranging from 12 % in the case of TAFP and PMFP to 3–5 % in the case of MEP and WDP.

Based on Fig. 2, a ranking is built to guide decision-makers in selecting midpoint indicators that can provide high environmental benefits at the expense of low supply chain costs when high priority (w value) to the environment criteria is presented in Table 1. Ranking 1 to 4 represents the midpoint indicators with achievable ERP and low economic investment. Ranking 5 to 7 represents environmental impacts that require high economic investment to reach high ERP. Finally, the last spot is reserved for ALOP since it requires high investment costs to reach a low ERP.

The results from Table 1 regarding the design of the supply chain for biobased PET production can be summarized as follow:

Table 1
Ranking of midpoint indicators and the trade-offs between ERP and SCTC considering high environmental priority ($w = 0.99$).

Ranking	Impact categories	ERP	SCTC
1	MEP	−4.5%	0.5%
2	WDP	−2.9%	0.6%
3	PMPF	−11.2%	2.7%
4	TAFP	−11.2%	3.0%
5	HTP	−27.5%	24.9%
6	FDP	−19.9%	23.1%
7	GWP	−19.3%	24.2%
8	ALOP	−8.0%	40.6%

a) *Easy to achieve*: It can reach the maximum possible gains for the MEP and WDP midpoint indicators with barely any additional supply chain costs.
b) *Quick wins*: There is the chance to make a significant impact (>10 %) in the TAFP and PMFP midpoint indicators with a relatively small (<5 %) increase in supply chain costs.
c) *High cost - high gain*: GWP, HTP, and FDP provide high environmental benefits; however, they come with a relatively high (>20 %) increase in the supply chain costs. At this point, an open discussion with decision-makers on the risks and benefits of considering these midpoint indicators is recommended (step 4 of the LCO framework, see Section 3).
d) *Too expensive*: ALOP evidenced relatively small environmental benefits with a very high increment in the supply chain cost. It is probably not worth focusing on this midpoint indicator from an economic perspective. However, land use is one of the most challenging issues that the production of biobased materials faces. Therefore, an extra effort (in terms of monetary support and incentives) should be considered to improve the current level of this indicator.

3.2. Trade-offs between economic and environmental criteria for selected impact categories

Optimal solutions are represented in Pareto frontiers for the environmental impacts that provide relatively high ERP with high SCTC – GWP, HTP, FDP, and ALOP. Fig. 3 presents the Pareto frontier for the GWP, whereas the other diagrams for other selected midpoint indicators are included in the Supplementary information. From the Pareto frontier, it is possible to extract the optimal solutions that could be interesting for decision-makers. However, some optimal solutions are clustered with others with similar environmental and economic performance. Interestingly, changes in the solutions (supply chain configurations) are marginal around a similar supply chain layout. Therefore, significant changes in the supply chain structure should be introduced to move to a new level of solutions. One optimal solution per cluster was selected to analyze the changes in the structure of different solutions in the Pareto frontier. The selection criterion was the lowest value of environmental impact (in this case, lowest GWP) within the cluster, as the focus is on providing solutions with the highest ERP. In Fig. 3, the environmental impacts for w values above 0.9 slightly change at the expense of significant changes in the supply chain costs, and therefore less clustered solutions are observed. For this reason, the solution with the lowest supply chain costs within this cluster was selected as an optimal solution.

It is helpful for decision-makers to understand what aspects of the supply chain change as the environmental priority increases since each selected optimal solution represents a specific supply chain configuration. For this purpose, a hotspot analysis of the selected optimal solutions is performed to identify the plants with the highest (and lowest) contribution to the ERP and SCTC. Each optimal solution among the selected w values (colored triangles in Fig. 3) is compared with the solution at the reference value ($w_{ref} = 0$). The results are calculated as a 'percentage (%) of change' between the reference solution and the environmentally improved one ($w > 0$). Then, the results are plotted in heat maps to show the low or high influence of the different plants on the economic and environmental performance of the biobased PET supply chain, as shown for GWP in Fig. 4. The same procedure is repeated for the HTP, FDP, and ALOP. The heat maps are included in the Supplementary information.

The red color represents a negative effect (low ERP) for the environmental criterion, while the green color represents a positive effect (high ERP). Overall, high priority to the environmental criteria positively influences all the nodes, as shown in Fig. 4A. As the environmental priority increases, plants F and M evidenced the highest ERP (41.7 % and 30 %, respectively). However, this behavior is almost constant for w values >0.1. Plants A and D significantly influenced the high environmental
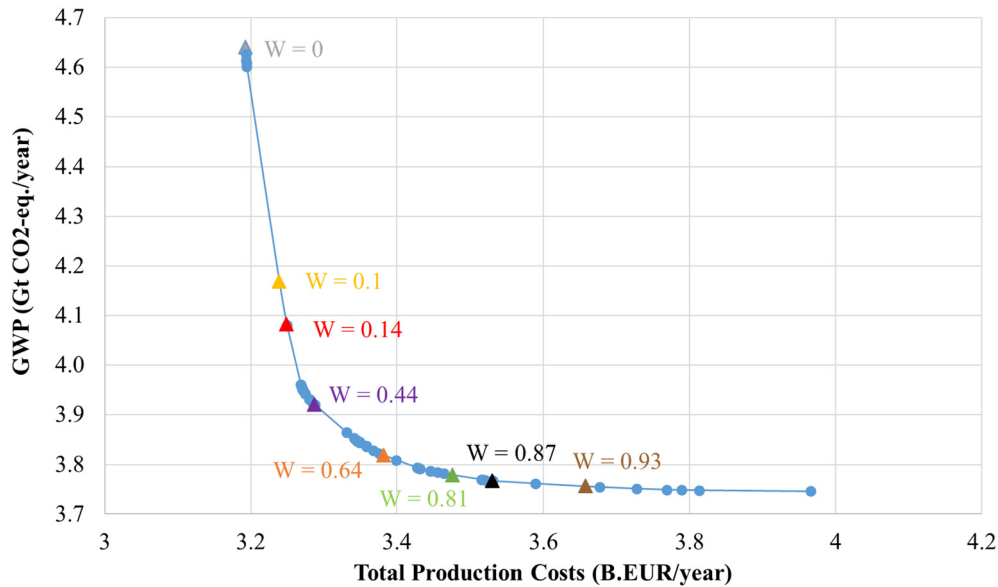
Fig. 3. Pareto frontier of the trade-offs between GWP and supply chain total costs. B.EUR/year = billion EUR per year.

prioritization, where the ERP increased to 26.6 % and 16.5 % compared to the reference case, respectively. Specific details of the supply chain configuration of Plant A are analyzed in Fig. 5 to understand the previous behavior. The main changes in the supply chain configuration are related to 1) the amount of product transported from different Plant A locations to Plant B and 2) the distances between them. First, Plant A, located in France, has a better GWP indicator (0.059 $kg\ CO_{2-eq.}$ /kg product) compared to other locations in Belgium (0.109 $kg\ CO_{2-eq.}$/kg product) and the Netherlands (0.152 $kg\ CO_{2-eq.}$/kg product). Therefore, the model decided to increase the product flow from Plant A, located in France, to Plant B at the expense of reducing the amount transported from Belgium and the Netherlands. Second, the shift to

A. Effect of weight on environmental criteria

	W = 0.10	W = 0.14	W = 0.44	W = 0.64	W = 0.81	W = 0.87	W = 0.93
Sugar Beet							
Miscanthus							
Plant A	0.2%	-12.3%	-12.3%	-13.9%	-24.6%	-23.7%	-26.6%
Plant B							
Plant C							
Plant D	0.0%	0.0%	0.0%	0.0%	-16.5%	-16.5%	-16.5%
Plant F	-47.9%	-40.4%	-41.7%	-41.7%	-41.7%	-41.7%	-41.7%
Plant M	-21.0%	-30.1%	-30.1%	-30.1%	-30.0%	-30.0%	-30.0%

Label   Low ERP   0% High ERP

B. Effect of weight on economic criteria

	W = 0.10	W = 0.14	W = 0.44	W = 0.64	W = 0.81	W = 0.87	W = 0.93
Plant A							
Plant B	-0.1%	28.1%	20.3%	20.3%	20.3%	96.1%	171.7%
Plant C							
Plant D	0.0%	0.0%	0.0%	0.0%	26.2%	26.2%	26.2%
Plant F	-4.9%	5.8%	6.4%	9.0%	12.9%	13.1%	17.6%
Plant M	40.3%	-6.9%	-6.9%	-6.9%	-6.7%	-6.7%	-6.7%

Label   High SCTC   0% Low SCTC

Fig. 4. Heat maps of the effect of the environmental priority (*w* values) in the % change of ERP (a) and the SCTC (b).

Reference case (W = 0)

Plant A
Location: France
Env. Impact: 0.059 kg CO2eq./kg product
Product Flow: 930.399 t/year

Plant A
Location: the Netherlands
Env. Impact: 0.152 kg CO2eq./kg product
Product Flow: 375.207 t/year

Total Distance: 1379 km

Total Distance: 360.3 km

Plant B
Location: Belgium

Plant A
Location: Belgium
Env. Impact: 0.109 kg CO2eq./kg product
Product Flow: 436.000 t/year

Total Distance: 187.4 km

W values > 0.81

Plant A
Location: France
Env. Impact: 0.059 kg CO2eq./kg product
Product Flow: 1.115.798 t/year ↑

Plant A
Location: the Netherlands
Env. Impact: 0.152 kg CO2eq./kg product
Product Flow: 31.560 t/year ↓

Total Distance: 1849 km ↑

Total Distance: 2.45 km ↓

Plant B
Location: Belgium

Plant A
Location: Belgium
Env. Impact: 0.109 kg CO2eq./kg product
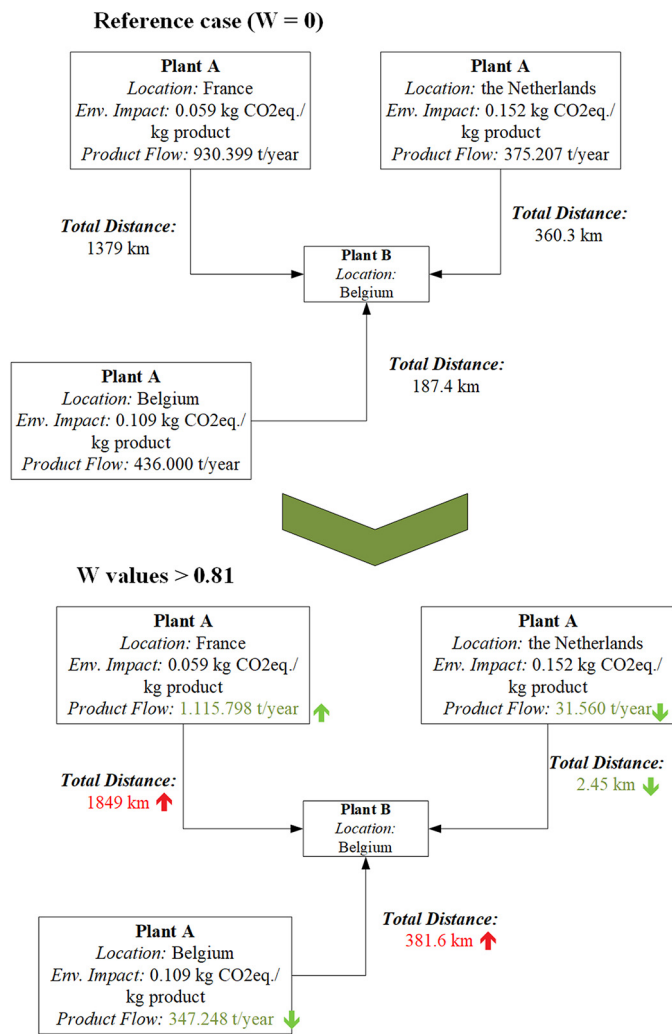*Product Flow:* 347.248 t/year ↓

Total Distance: 381.6 km ↑

Fig. 5. Main changes in the supply chain configuration of plant A for the environmental criteria as the environmental priority increases. The main changes in the supply chain are highlighted in red.

supply products from plant A in France to plant B in Belgium increased the total transportation distance compared to the reference case. However, this increment has a low influence on the network design since environmental impacts from transportation represent 25 % of the total supply chain environmental impact (see Fig. 6).

Regarding the improvement in the ERP of Plant D, the net benefit comes from reducing the supply of products from plant D located in Germany (higher environmental impact - 0.282 $kg\ CO_{2-eq.}$/kg product), and the opening of plant D in the United Kingdom (UK) with lower environmental impact (0.228 $kg\ CO_{2-eq.}$/kg product), as described in Fig. 7. There is an increment in the transportation distance from plant D in the Netherlands and UK. At the same time, there is a reduction in the transportation distance between plant D, located in Belgium and Germany, to the demand around Europe.

The red color represents a negative effect (high SCTC) for the economic criterion, while the green color represents a positive effect (low SCTC). The supply chain costs of plant M were reduced up to 7 % for w values >0.1 due to the selection of plants with 1) lower production cost (and better environmental performance) and 2) shorter transportation distances, as described in Fig. 8. In the reference case, plant M in Poland supplies approx. 15 % of the total product required in plant D with a production cost of 210.4 €/t. As the environmental priority increases (w values >0.1), the model selects a plant M location (in Belgium) with better environmental performance (and even lower production costs). However, the positive effect evidenced in plant M comes at the expense of increasing the SCTC of plant F since a location (Italy) with higher production costs (263.1 €/t) and a longer transportation distance was selected. Additionally, the environmental performance of plant F in Italy is lower than plant F in Sweden, so the ERP of plant F in Fig. 4 remains almost unchanged.

A negative effect (high SCTC) was evidenced in plant B as the environmental priority increased, reaching the worst value at $w = 0.93$ (see, Fig. 9). In the reference case, plant B in France supplies products for two plants C in Belgium and the Netherlands. As the environmental priority increases, the model opens other plant B locations with better environmental performance and shorter transportation distances. However, in the reference case, plants B-2 and B-3 incurred higher production costs (134.4 and 142.1 €/t, respectively) than plant B in France (97.7 €/t). Therefore, we can see an improvement in the ERP of plant B at the expense of increasing the supply chain costs up to 171 %.
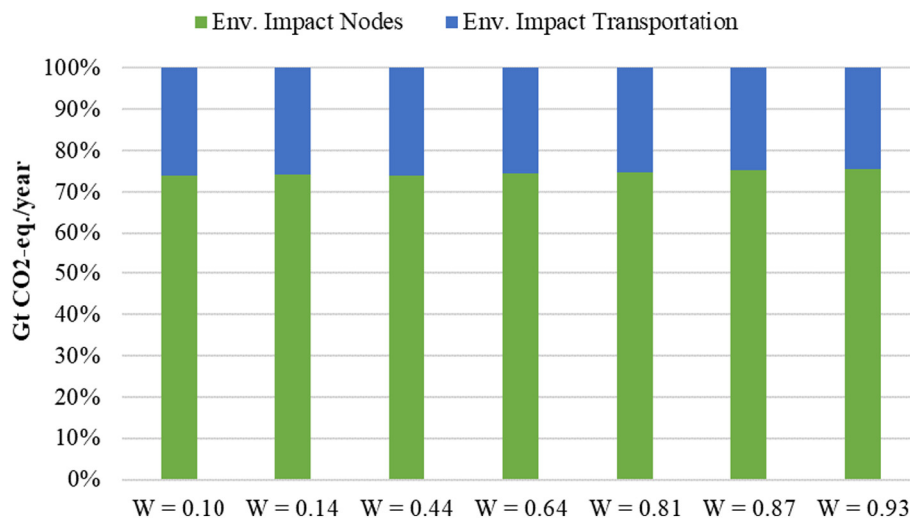

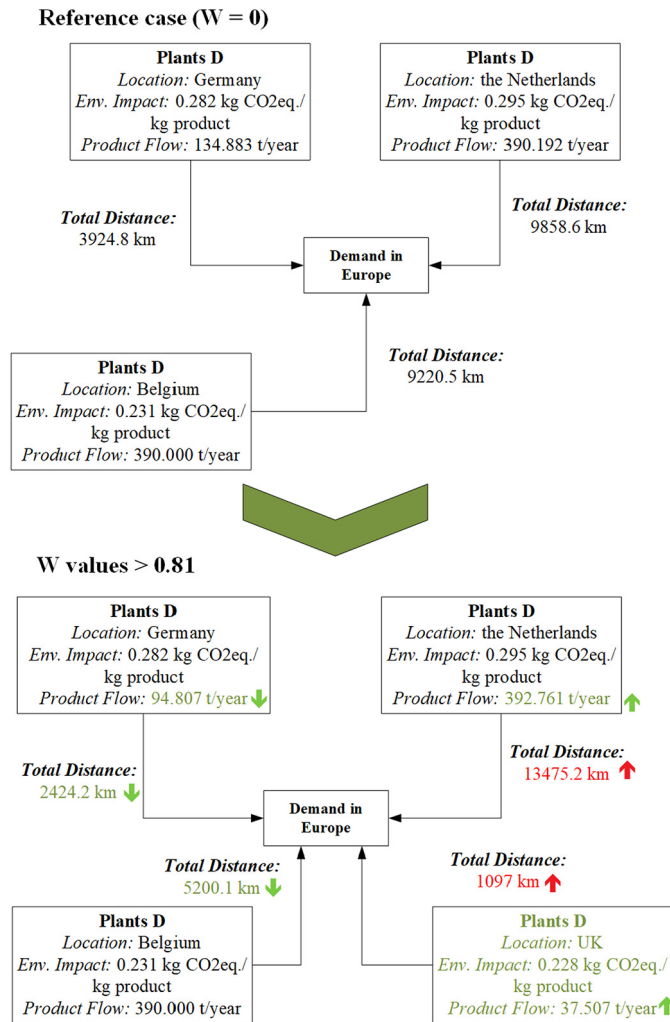**Fig. 6.** Distribution of the total environmental impact between nodes and transportation.

Fig. 7. Main changes in the supply chain network of plant D for the environmental criterion as the environmental priority increases. The main changes in the supply chain are highlighted in red.

Fig. 8. Main changes in the supply chain network of plant M for the economic criterion as the environmental priority increases. The main changes in the supply chain are highlighted in red.

consequences on the three main areas of concern: human health, ecosystems, and resources. Our results suggest that if manufacturers give an environmental priority of at least 10 % ($w = 0.1$) in the design of

4. Discussion

The chemical sector has set some ambitious sustainability goals, mostly related to reducing GHG emissions (IEA, 2020). Besides the importance of measuring and reducing GHG emissions from industrial processes, the new generation of biobased chemicals should focus on broader environmental impacts from manufacturing these new products and preventing the high amount of pollutants that the chemical industry has created since the 19th century (Hoffmann, 1993). One crucial aspect (highlighted in this study) is the accountability of critical environmental impacts (human toxicity, land use, fossil depletion, acidification) in the design of supply chains for these biobased chemicals. Although, economic incentives for producing these biobased chemicals should not be excluded as the current economic model relies on the balance between the demand and supply model. Interesting conclusions can be drawn from the trade-offs between the economic and environmental criteria for biobased PET production. The European Commission (EC) supports the chemical industry in the transition to the manufacture and design of sustainable chemicals (European Commission, 2020). Therefore, biobased PET manufacturers (willing to adhere to this directive) could improve the environmental impact of their supply chain with low investment costs. Climate change, human toxicity, and fossil depletion are getting more attention due to the direct
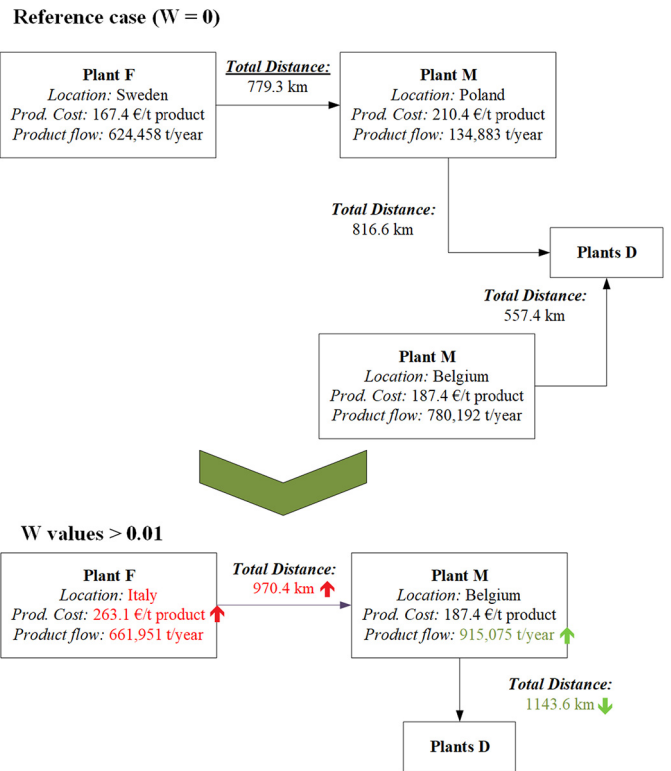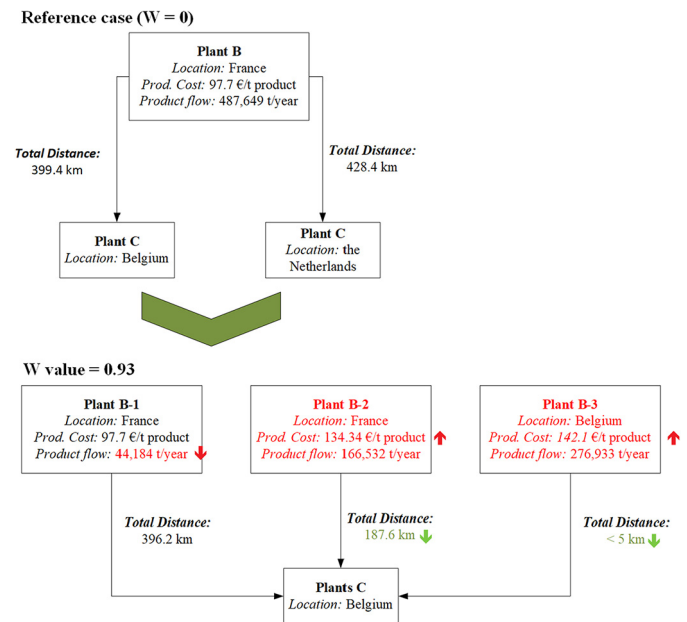

Fig. 9. Main changes in the supply chain network of plant B for the economic criterion as the environmental priority increases. The main changes in the supply chain are highlighted in red.

supply chains, there will be an environmental reduction in GWP of up to 12 %. Similarly, an increase of up to 20 % ($w = 0.2$) of the environmental priority could provide environmental reductions of approx. 12 %, 15 % and 20 % for the FDP, GWP, and HTP, respectively. These environmental benefits will come at the expense of low investment costs (up to 2 %), as shown in Fig. 2. However, the reduction of GWP, HTP, and FDP for designing supply chains considering high environmental priority ($w = 0.9$) came at the expense of high investment costs (>20 %). From our results, it is clear how the EC can support the chemical and biobased chemical industries to increase their commitment to reducing environmental impact by designing supply chains that account for critical environmental categories (e.g., GWP, HTP, FDP) with low investment costs. Nevertheless, manufacturers will not be encouraged to improve their supply chains unless the EC proposes clear directives and policies to guide these industries.

Land use is a cornerstone topic in the future development of biobased chemicals from first-generation (food crops) and (even) second-generation (lignocellulosic biomass) feedstocks. This study shows how the low environmental gains from improving the ALOP of the supply chain for biobased PET production required high investment costs. The high costs are attributed to the high production costs of sugar beet and *miscanthus* in the locations where low ALOP was estimated. However, the environmental performance did not significantly improve (<8 %). Therefore, using non-crop feedstocks and improving technological techniques for *miscanthus* cultivation (e.g., improving fertilization techniques) might provide better environmental gains in ALOP with lower investment costs.

From a strategic point of view, manufacturers need to know which section of the supply chain should be improved to reach specific environmental targets. This study proposes a simple tool (hotspot analysis) to detect the plants within the supply chain that contribute most to the environmental and economic criteria. Manufacturers can see how the performance of the supply chain changes at different levels of environmental priority. Moreover, a detailed analysis of the supply chain configuration can be done by analyzing the mass flow distributions, environmental impacts per midpoint indicator, and production costs. It is important to highlight that this process is not automatic (at the moment) since this study wanted to analyze how changes in the environmental priority influence specific aspects of the supply chain and the effect on economic and environmental performance. Therefore, this study 'paves the way' to foster the development of frameworks/interfaces to facilitate the (automatic) selection of supply chain configurations by changing the environmental priority (taken here as a value between 0 and 1).

The transition to the future biobased chemical industry should come along with the awareness of the potential environmental impacts of producing these chemicals. This study proposes accounting for the environmental impacts in the design of supply chains using (problem-oriented) midpoint indicators. These indicators have not been widely studied in optimization modeling due to the inherent complexity of understanding the "meaning" of designing supply chains using midpoint indicators that describe "one part of the whole" cause-effect chain, described in the introduction section. The optimization modeling of supply chains where total costs are compared to different midpoint indicators (e.g., the 17 categories in the ReCiPe method) is demanding. From this point of view, it might be convenient to use endpoint indicators that are easy to explain to decision-makers and the general public since they evaluate the effect of emissions of a particular product or process to the end of the cause-effect chain (Hauschild et al., 2017). However, midpoint indicators should not be discarded from the decision-making process, mainly if the assessment is performed from the manufacturer's or producer's point of view. This study shows how the use of rankings for enlisting midpoint indicators can foster the design of environmentally-improved supply chains to reach specific companies' sustainability targets (e.g., reduction of water use and acidification). Simultaneously, the ranking provides insights to the manufacturers on

potential environmental benefits in the design of supply chains to communicate with decision-makers. The ranking aims to foster policies that support companies in the transition to design environmentally-improved supply chains (e.g., improving the environmental performance of plants/suppliers located in countries with low production costs).

The proposed model in this paper has limitations in how the model was built (assumptions) and data availability. The model required detailed data on technical (plant locations, distances between plants, processing capacity, among others), economic (capital and operating costs of plants, feedstock and reagents costs, freight costs, among others), and environmental (environmental impacts of plants and transportation) aspects. Technical data of the different plants were collected from the existing infrastructure of the primary chemical producers (e.g., ethylene plants) in Europe through a web search. However, some plants needed to be "virtually" designed since no physical infrastructure was available. For this purpose, the virtual location approach proposed by Kozlo et al. (2018) was used. However, this approach still attains uncertainty compared to the commercial data used for the other plants. Economic data were mainly modeled using the approach proposed by de Jong et al. (2015) since access to accurate commercial data was limited. Detailed data for the environmental assessment of different plants/suppliers in different countries were required. For example, there were limited data on the environmental impact of sugar beet and *miscanthus* cultivation in different EU countries. General data about the cultivation of these two crops were available (in databases and scientific publications) for a group of countries i.e. Belgium (Belboom and Léonard, 2016), Greece (Foteinis et al., 2011), Germany (Wagner et al., 2019), the Netherlands (Smit et al., 2010), Poland (Krzyżaniak et al., 2020; Przyby, 2011), United Kingdom (Renouf et al., 2008; Shemfe et al., 2016). However, specific data (e.g., differences in fertilization techniques, irrigation, pesticides, etc.) per EU country were scarce. In this sense, regionalized LCA modeling is required more than ever (Frischknecht et al., 2019) to overcome the challenges of data requirements.

Finally, midpoint indicators address different issues, i.e., GWP accounts for the effects of increasing the concentration of GHG (namely carbon dioxide, methane, and nitrous oxide) in the warming of the atmosphere. At the same time, categories such as ALOP measure the change in land use and its effect on species loss (Huijbregts et al., 2017). However, understanding the significance of these midpoint indicators can (still) be challenging for decision-makers. Therefore, future research could focus on a lower analysis level, including the elementary flow inventory instead of midpoint indicators in the optimization model for designing supply chains. The main advantage could be the possibility to identify (through hotspot analysis) the main stages where specific elementary flows have the highest contribution and therefore be able to propose concrete solutions (e.g., using a different type of fertilizer) for improving the contribution of these elementary flows. However, more complexity is added to the model since more criteria are included, i.e., from 9 midpoint indicators used in this study to approx.—4000 elementary flows as included in the ecoinvent database (Ecoinvent, 2020).

5. Conclusion

Previous studies showed how the production of biobased PET had a better environmental impact in terms of GWP than fossil-based PET. However, biobased PET performed worse in other midpoint indicators, such as HTP, FDP, and ALOP. Therefore, accounting for these midpoint indicators (that could hinder the overall environmental performance of biobased PET) in the design of supply chains is more relevant than ever. This paper evaluated the contribution of midpoint indicators (e.g., GWP, HTP, FDP, WDP, MEP, and ALOP) as environmental criteria in the design of supply chains through a life cycle optimization framework. Using the production of biobased PET as a case study, we showed how it is possible to reduce the environmental impact (for some

midpoint indicators) without increasing the total supply chain costs. From the trade-off analysis between environmental and economic criteria, critical midpoint indicators (GWP, HTP, FDP, and ALOP) were identified that provided higher environmental reduction gains at the expense of high investment costs of the supply chains. The hotspot analysis supported identifying critical stages (processing plants) that influence the economic and environmental performance of the supply chain configurations. Our study shows that a broader spectrum of environmental impacts rather than only GHG emissions should be included when designing sustainable biobased supply chains, despite the challenges of understanding the impact of the environmental midpoint indicators on the decision-making process. This paper aimed to provide detailed insights on how to reduce the environmental impact of PET value chains at which costs levels for the involved companies and other decision-makers. Further research on better ways to harmonize data collection of the different actors (suppliers, processors, and customers) throughout the PET value chain should be considered.

Data availability

The data that support the findings of this study are openly available in Zenodo at https://doi.org/10.5281/zenodo.6751224 and https://doi.org/10.5281/zenodo.6751430.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A

Nomenclature list

The multi-echelon supply chain is represented by a graph $G = (V,A)$, where V represents the set of nodes, and A denotes the set of arcs between these nodes. The set of nodes is further divided into different subsets, referring to the different supply chain entities (see notation below). Let $\delta^-(i)$ and $\delta^+(i)$ be the set of all incoming and outgoing arcs for node i, respectively. Note that arcs are only defined between two consecutive supply chain echelons, as depicted in Fig. 1. This means, e.g. that all outgoing arcs for nodes $i \in V^A$ are incoming arcs for nodes $j \in V^B$ etc.

Sets

V set of all network nodes, indexed by i or j. $V = V^S \cup V^A \cup V^B \cup V^C \cup V^D \cup V^F \cup V^M$ with

V^S set of all supply regions
V^A set of all ethanol plants
V^B set of all ethylene plants
V^C set of all EG plants
V^D set of all PET plants
V^F set of all fast pyrolysis plants
V^M set of all PTA plant

A set of all arcs, indexed by a. Each $a \in A$ is defined as (i,j) with $i,j \in V$ and $i \neq j$.
$\delta^+(i)$ set of all arcs leaving node i.

$\delta^-(i)$ set of all arcs entering node i.
E set of all environmental impact categories (such as Global Warming Potential, Human Toxicity Potential, Fossil Depletion Potential, Agricultural Land Occupation Potential, among others), indexed by e.

Parameters

c_i^B unit supply cost of sugar beet from node $i \in V^S$.
c_i^M unit supply cost of miscanthus from node $i \in V^M$.
q_i^B supply quantity of sugar beet available at node $i \in V^S$.
q_i^M supply quantity of miscanthus available at node $i \in V^M$.
Q_i capacity of node $i \in V \backslash V^S$.
c_i^P unit operational cost for node $i \in V \backslash V^S$.
p^C price for a unit of co-product (sugar beet pulp) on the market.
c_a^T unit transport cost on arc a.
f_i^V fixed cost of activating node i in the supply chain network.
f_a^T fixed transport cost for activating arc a.
d_a length (distance) of arc a.
ε_e^T environmental impact per category e of transporting per item per distance unit.
ε_{ei}^P environmental impact per category e for producing one unit in plant i.
γ_i conversion factor for main product at node $i \in V \backslash V^S$.
γ_i^{SBP} conversion factor for sugar beet pulp obtained as co-product from plant $i \in V^A$.
γ_i^C proportion of main product from plant C in final product of plant D.
γ_i^M proportion of main product from plant M in final product of plant D.
M an arbitrary large value. A value equal to $\max_i\{Q_i\}$ is sufficiently large.
D total demand for pre-form PET.

Decision variables

y_i binary variable $= 1$, if node $i \in V \backslash V^S$ is activated; 0, otherwise.
t_a binary variable $= 1$, if arc is activated; 0 otherwise.
x_a^B supply quantity of sugar beet on arc $a \in \delta^+(i)$, $i \in V^S$.
x_a^M supply quantity of miscanthus on arc $a \in \delta^+(i)$, $i \in V^S$.
x_a the quantity transported on arc $a \in \delta^+(i)$, $i \in V \backslash \{V^S \cup V^D\}$.
x_i^P the quantity of main product produced at plant $i \in V \backslash V^S$.
x_i^{SBP} the quantity of sugar beet pulp obtained as co-product from plant $i \in V^A$.

Appendix B. Supplementary Information

Supporting Information S1: This supporting information provides details of the trade-offs between the economic (total supply chain costs) and the environmental (environmental reduction potential) criteria for selected impact categories, such as Human toxicity potential, Fossil depletion potential and Agricultural Land Occupation Potential. Supplementary data to this article can be found online at https://doi.org/10.1016/j.spc.2022.10.015.

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