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# Design of biobased supply chains on a life cycle basis: A bi-objective optimization model and a case study of biobased polyethylene terephthalate (PET)

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ABSTRACT

Bioplastics are considered a sustainable alternative to (partly) substitute fossil-based plastics. Nevertheless, it is still uncertain if the use of biomass for the production of bioplastics can mitigate the environmental impact of fossil-based plastics and simultaneously provide economic benefits. An optimization model is proposed to design biobased supply chain networks that account for economic (total costs) and environmental (greenhouse gas emissions) criteria. Life cycle costing and life cycle assessment were used to evaluate the economic and environmental costs of the biobased polyethylene terephthalate (PET) production using sugar beet and wheat as feedstock. The 100% biobased PET production evidenced higher economic and environmental costs than the 30% biobased PET production. The feedstock selection played a key role, whereas the use of wheat for both 30% and 100% biobased PET had the highest costs and greenhouse gas emissions. It is highlighted that the economic performance of the biobased terephthalic acid (PTA) production, the feedstock selection (sugar beet), and the carbon tax scenario (>100 €/t $CO_2$) are key parameters for designing a sustainable biobased PET supply chain.



## 1. Introduction

In 2018, the European Commission (EC) published the roadmap for a sustainable bioeconomy in Europe, highlighting the importance of the bioeconomy for the future development of Europe and the transition to a low-carbon economy. The bioeconomy sector had a total turnover of € 2.3 trillion, where the manufacture of biobased chemicals and plastics accounted for € 177 billion (European Commission, 2018). Despite the several benefits of the European bioeconomy, some limitations still hinder its full implementation. For example, the success of the biobased chemicals and plastic sector depends on the lobbying efforts of governmental agencies looking for incentives or regulations for the production of biobased products (Lewandowski, 2017). On the other hand, there is a discussion on the environmental benefits of biobased products compared to fossil-based ones. Biobased products perform better in terms of GHG emissions; however, they tend to underperform in other categories namely, water use, land use, biodiversity loss, and eutrophication ((Garcia-Velasquez and van der Meer, 2021)). Despite these bottlenecks, the EC encourages new value chains and greener, more cost-effective industrial processes to support the modernization and strengthening of the EU bioeconomy (European Commission, 2018). Therefore, decision-makers and governmental entities need tools to start acting towards setting biobased value chains that promote the creation of local jobs and provide incentives to industries promoting the shift from fossil-based to biobased products.

The design of biomass supply chains for the production of biobased materials requires the decision-maker to know the possibilities, alternatives, or scenarios that provide processes with the best economic, environmental and social performance (Cambero and Sowlati, 2014). A supply chain is defined as a combination of processes to fulfill customers' requests, including different entities from suppliers, transporters, manufacturers, and distributors, among others (Barbosa-Póvoa et al., 2018). Supply chain design is traditionally linked to meeting the customer's demands at the minimum cost; however, the concept has expanded over time by including other criteria, such as minimizing the environmental and social impact. According to (Barbosa-Póvoa et al., 2018), the most studied criteria in the supply chain design are economic and environmental; however, the social criterion is attracting attention through the Sustainable Development Goals (SDG). The most used

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**Nomenclature**

$g$ as co-products
$i, j$ as entities
$m$ as feedstock
$n$ as capacity of entities
$s$ as means of transport
$r$ as feedstock supplier

Sets
$G$ as co-products in entities, $g \in G$
$M$ as type of feedstock, $m \in M$
$R$ as regions, $r \in R$
$S$ as transportation mode, $s \in S$

*Each level of the supply chain is defined by one kind of entity (Plant A, Plant B, Plant C, and Plant D) and therefore, we have the following sets:*
$Pa$ as location plant A, $i \in Pa$
$Pb$ as location plant B, $i \in Pb$
$Pc$ as location plant C, $i \in Pc$
$Pd$ as location plant D, $i \in Pd$
$Pm$ as location plant M, $i \in Pm$
$D$ as location demand, $i \in D$
Set: $I = Pa \cup Pb \cup Pc \cup Pd \cup Pm \cup D$ contains all entities

*For each entity, there is also a size category set:*
$PaSz$ as size of plant A, $n \in PaSz$
$PbSz$ as size of plant B, $n \in PbSz$
$PcSz$ as size of plant C, $n \in PcSz$
$PdSz$ as size of plant D, $n \in PdSz$
$PmSz$ as size of plant M, $n \in PmSz$
Set: $N = PaSz \cup PbSz \cup PcSz \cup PdSz \cup PmSz$ contains all entities sizes

Parameters
$B^{avail}_{m,r}$ availability of feedstock $m$ in region $r$, $m \in M$ and $r \in R$
$C_i$ capacity plant $i$, $i \in I$
$CAP_{m,i,n}$ capital costs of plant $i$ and size $n$ using feedstock $m$, $i \in Pa$, $m \in M$ and $n \in PaSz$
$CAP_{i,n}$ capital costs of plant $i$ and size $n$, $i \in I$ and $n \in N$
$Y^{product}_i$ conversion yield of product in plant $i$, $i \in I$
$Y^b_{m,i}$ conversion yield of feedstock $m$ in plant $i$, $m \in M$, $i \in Pa$
$OP^{fix}_{m,i,n}$ fixed operative costs of plant $i$ and size $n$ using feedstock $m$, $i \in Pa$, $m \in M$ and $n \in PaSz$
$OP^{fix}_{i,n}$ fixed operative costs of plant $i$ and size $n$, $i \in I$ and $n \in N$
$T^{fix}_{r,s}$ fixed transportation costs in region $r$ with transportation mode $s$, $r \in R$ and $s \in S$
$T^{fix}_{i,s}$ fixed transportation costs from plant $i$ with transportation mode $s$, $i \in I$ and $s \in S$
$E_s$ GHG emissions from transportation mode $s$, $s \in S$
$E_{m,i}$ GHG emissions from the life cycle of the product in plant $i$ using feedstock $m$, $i \in Pd$ and $m \in M$
$\$^{co-prod}_{m,g,i}$ selling price of co-product $g$ from feedstock $m$ in plant $i$, $i \in I$, $m \in M$ and $g \in G$
$B^{cost}_{m,r}$ supply cost of feedstock $m$ in region $r$, $m \in M$ and $r \in R$
$Z_{r,i,s}$ transportation distance from region $r$ to plant $i$ with transportation mode $s$, $r \in R$, $i \in Pa$ and $s \in S$
$Z_{i,j,s}$ transportation distance from plant $i$ to plant $j$ with transportation mode $s$, $i \in I$, $j \in I$, and $s \in S$
$OP^{var}_{m,i,n}$ variable operative costs of plant $i$ and size $n$ using feedstock $m$, $i \in Pa$, $m \in M$ and $n \in PaSz$
$OP^{var}_{i,n}$ variable operative costs of plant $i$ and size $n$, $i \in I$ and $n \in N$
$T^{var}_{r,s}$ variable transportation costs in region $r$ with transportation mode $s$, $r \in R$ and $s \in S$
$T^{var}_{i,s}$ variable transportation costs from plant $i$ with transportation mode $s$, $i \in I$ and $s \in S$

Scalars
$\$^{carbon\ tax}$ carbon tax pricing – *25, 50, 100, 150 €/t $CO_2$*
$NPa$ number of plants A – *50*
$NPb$ number of plants B – *21*
$NPc$ number of plants C – *9*
$NPd$ number of plants D – *9*
$NPm$ number of plants M – *6*
$Z^{co-prod}$ transportation distance co-product - *100 km*
$W^{EG}$ weight fraction of EG to produce PET – *0.3 kg EG/kg PET*
$W^{PTA}$ weight fraction of PTA to produce PET – *0.7 kg PTA/kg PET*

Variables

Binary Variables
$up_{i,n}$ binary variable for plant $i$ and size $n$, $i \in I$; $n \in N$; $up_{i,n} \in \{0, 1\}$

*Continuous variables*
$x^{co-prod}_{g,i}$ mass flow of co-product $g$ from plant $i$, $g \in G$ and $i \in I$
$x^b_{m,r,i}$ mass flow of feedstock $m$ in region $r$ to plant $i$, $m \in M$, $r \in R$ and $i \in Pa$
$x^{product}_{i,j}$ mass flow of main product from plant $i$ to plant $j$, $i \in I$ and $j \in I$

metrics within the economic criteria are the total costs, profits, and Net Present Value (NPV). In contrast, the environmental criteria cover metrics such as carbon dioxide ($CO_2$) emissions assessed as carbon footprint and greenhouse gas (GHG) emissions.

The selection of the best criteria should consider the public awareness of sustainability issues, which can boost decision-makers to understand the life cycle impact of the evaluated biomass supply chain on economic and environmental aspects (Sharma et al., 2013). For this purpose, Operational Research (OR) has emerged as a discipline that follows the optimization paradigm and helps the decision-maker select the key criteria that will influence the overall quality of the decisions (Azapagic and Clift, 1999). Among the different OR methods, optimization is commonly used to address the design of supply chains where the optimization problem is expressed as an objective function that includes decision variables and parameters to maximize or minimize according to the necessity of the problem (Cambero and Sowlati, 2014). Total costs seem to be the best metric to optimize and maybe the most convenient; however, the emphasis has changed towards multiple criteria to establish trade-offs between alternatives and consequences (Saarikoski et al., 2016). Economic and environmental criteria have become prevalent due to the possibility of generating a portfolio of possible solutions for decision-makers that could select the best option based on their needs (Cambero and Sowlati, 2014; Capitanescu et al., 2016). Nevertheless, decision-makers face challenges when presented with multiple criteria choices for selecting the best supply chain. First, decisions are subjective to the motivations or drivers of the decision-maker, who may not understand the trade-offs between the different criteria. Furthermore, a product with higher production costs and better environmental performance will not be considered due to the low economic performance (Tarne et al., 2019). Other approaches consider the design of biomass supply chains using carbon-pricing policies to account for the environmental impact of specific products or processes (Waltho et al., 2019). Different carbon-pricing policies are applied to set a price or trade system to reduce GHG emissions from products or processes. The most popular policies are the carbon tax, carbon cap, trade-and-cap, and carbon offset (Waltho et al., 2019).

GHG emissions are classified into three scopes: Scope 1 emissions are primarily linked to company facilities and the use of different transportation mediums, whereas scope 2 emissions are related to the purchase of electricity, steam, heating, and cooling. Finally, scope 3 emissions are related to upstream (feedstock acquisition and transportation) and downstream (processing and transformation, usage phase, and end-of-life) activities (Barrow et al., 2013). According to the GHG protocol, companies must report direct GHG emissions (scope 1), while the reporting of emissions from the upstream and downstream processes (scope 3) is voluntary, but it is strongly encouraged by environmental organizations (Ranganathan et al., 2015). Emissions from transportation are widely included in the design of biomass supply chains with different carbon-pricing policies, whereas emissions from the product life cycle (upstream and downstream) have not been considered. At the corporate level, scope 3 emissions are calculated from process-based life cycle assessment (LCA) (Hertwich and Wood, 2018). Despite the high contribution (>80%) of scope 3 emissions to the overall GHG inventory, LCA approaches are not widely used within the design of biomass supply chains because of the high data requirements to perform the assessment (Waltho et al., 2019).

The environmental performance of biobased products (e.g., biobased chemicals) has been evaluated using life cycle assessment (LCA) tools (Gomes et al., 2019; Liptow et al., 2015; Volanti et al., 2019). However, the design of biomass supply chains has mostly focused on producing biofuels and electricity from renewable resources (e.g., agricultural products and waste) (Ba et al., 2016; Malladi and Sowlati, 2020). (Dessbesell et al., 2017) reviewed the available literature on the design of biomass supply chains, concluding that only 5% of the reviewed papers (3 out of 59 papers) considered the supply chain for biobased materials and chemicals production. Since then, the interest in designing supply chains to produce biobased materials and chemicals has been increasing as reported in different publications (Balaman et al., 2018; Galanopoulos et al., 2019; He-Lambert et al., 2019). Regarding the used criteria, most of the publications on the topic "biobased supply chain" focused on the supply chain design using a single criterion - production costs (Galanopoulos et al., 2019; He-Lambert et al., 2019; Panteli et al., 2017). In contrast, few publications included environmental dimensions as an objective function in the optimization model (Balaman et al., 2018; Jonkman et al., 2019). As climate change policies are increasingly promoting technologies for GHG-emission reduction and bioplastics hold a promise to reduce GHG emissions in the plastics sector, it is highly relevant to include environmental criteria in the supply chain optimization.

This paper aims to develop an optimization model for the design of biobased supply chains using carbon-pricing policies (specifically, a carbon tax) to account for GHG emissions in economic terms. The tool can be used as a guideline for decision-makers in selecting the supply chain configurations, accounting for GHG emissions from the transportation network and production process using the LCA methodology. The production of biobased PET (polyethylene terephthalate) using sugar beet and wheat as feedstock was selected as a case study. A single-objective optimization model was proposed involving two criteria: total production costs and environmental costs. The model correlates the biomass availability and supply logistics with the PET demand to design a cost-effective supply chain that accounts for environmental impacts (GHG emissions) of biobased PET production based on our previous work (Garcia-Velasquez and van der Meer, 2021). The economic criterion involves calculating the production costs using the Life Cycle Costing (LCC) framework. In contrast, the environmental criterion accounts for GHG emissions from the LCA into monetary values using carbon-pricing policies (e.g., carbon tax).

This paper is structured as follows: the model characterization (from the problem definition, model formulation, model constraints to the single-objective approach), description of the case study, methodologies used (LCA and LCC), and other considerations (carbon tax) are described in **Section 2**. Afterward, the main outcomes of the optimization model are presented in **Section 3**. The limitations and future research are discussed in **Section 4.** Finally, **Section 5** presents the main conclusions of the design of the biobased supply chain for biobased PET production.

## 2. Methods

### *2.1. Model characterization*

#### *2.1.1. Problem definition*

The supply chains for biobased and fossil-based polymers have not addressed the environmental costs in their design. Therefore, this paper aims to integrate the environmental costs into the economic model for designing the supply chain network at a strategic-decision level for biobased PET production using the *BeWhere* model. This model is a spatially-explicit mixed-integer linear program (MILP) widely used in optimization studies for bioenergy production (Khatiwada et al., 2016; Leduc, 2009; Mandova et al., 2018). The model minimizes the costs of the entire supply chain, including feedstock production and transportation, processing, and product transportation. GHG emissions were calculated with LCA (Garcia-Velasquez and van der Meer, 2021), and the costs for emitting/mitigating GHG emissions are included in the model using carbon-pricing policies (e.g., carbon tax) (World Bank, 2019).

The optimization model is defined as follows:

*Given*

- The availability of feedstock and the location of the suppliers
- Feedstock cost per supplier location
- The location of supply chain entities (e.g., processing plants)
- Investment costs
- Operating costs (e.g., reagents costs, utility costs, labor costs)
- Transportation distances between the entities
- Transportation costs (fixed and variable) for different transport modes
- Maximum and minimum flow capacities
- Maximum and minimum acquisition and production capacities
- Processing efficiency in each entity
- Market prices of products
- GHG emissions factors from the LCA
- GHG emissions factors for the different transportation modes
- Carbon tax
- Demand location and volume

*Determine*

- The supply chain network configuration (feedstock suppliers and entities)
- The flow amounts between supply chain entities
- The product cost in the supply chain entities

*So as to*

- Minimize the global supply chain costs
- Determine the effect of GHG emissions on the supply chain costs

The developed model is described in detail in the next sections.

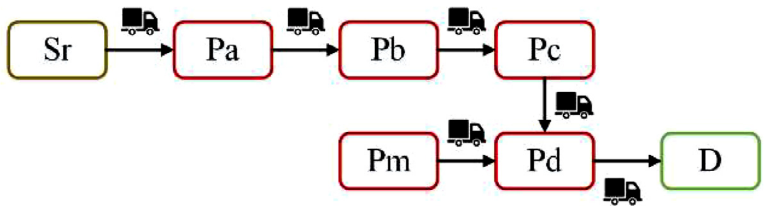


**Fig. 1.** Schematic representation of the supply chain network.

### 2.1.2. Model formulation

The supply chain involves a three-stage echelon structure: feedstock suppliers, processing plants, and demand, as presented in Fig. 1. $S_r$ represents the feedstock supplier, $P_A$ the plant A, $P_B$ the plant B, $P_C$ the plant C, $P_D$ the plant D, $P_M$ the plant M and $D$ the demand.

The definition of sets, variables, and parameters of the model are presented in the nomenclature list. The description of the constraints and objective function is presented below. The optimization model has as its main objective the total costs distributed between production and environmental costs. The constraints are grouped into four groups: feedstock availability, capacity constraints (entities and feedstock suppliers), mass balance, and operational constraints, such as the number of available entities.

### 2.1.3. Model constraints

This section presents the model constraints as characteristics that need to be guaranteed for the supply chain network design.

$$\sum_{i\in Pa} x^{b}_{m,r,i} \leq B^{avail}_{m,r} \qquad \forall\ m \in M,\ \forall\ r \in R \tag{1}$$

Eq. (1) assures that the amount of feedstock to be supplied to the first processing plant A is lower than the feedstock available. Where, $x^{b}_{m,r,i}$ is the amount (mass) of feedstock $m$ from region $r$ to plant A and $B^{avail}_{m,r}$ is defined as the remaining feedstock that can be potentially used to produce biobased materials (see Eq. (2)) when the demand for food and feed is supplied. The feedstock trade (exports and imports) was an important factor in increasing or decreasing biomass availability.

$$B^{avail}_{m,r} = B^{productivity}_{m,r} + B^{import}_{m,r} - B^{food}_{m,r} - B^{feed}_{m,r} - B^{export}_{m,r} \qquad \forall\ m \in M,\ \forall\ r \in R \tag{2}$$

Where,

$B^{productivity}_{m,r}$ is the amount of feedstock $m$ produced in region $r$
$B^{import}_{m,r}$ is the imported feedstock $m$ in region $r$
$B^{food}_{m,r}$ is the amount of feedstock $m$ for food supply in region $r$
$B^{feed}_{m,r}$ is the amount of feedstock $m$ for feed supply in region $r$
$B^{export}_{m,r}$ is the exported feedstock $m$ in region $r$.

*Capacity constraints*

$$\sum_{m\in M}\sum_{r\in R} x^{b}_{m,r,i} \leq \sum_{n\in PaSz} C_i * up_{i,n} \qquad \forall\ i \in Pa \tag{3}$$

$$\sum_{j\in J} x^{product}_{i,j} \leq \sum_{n\in N} C_i * up_{i,n} \qquad \forall\ i \in I \tag{4}$$

$$\sum_{j\in Pc} x^{product}_{i,j} * W^{EG} + \sum_{j\in P_M} x^{product}_{i,j} * W^{PTA} \leq \sum_{n\in SzPd} C_i * up_{i,n} \qquad \forall\ i \in P_D \tag{5}$$

$$\sum_{j\in Pd} x^{product}_{i,j} \leq C_i \qquad \forall\ i \in D \tag{6}$$

**Equations (3 – 6)** describe the mass flow limitations between the suppliers and processing plants. The amount of feedstock $m$ supplied to Plant A should not exceed its capacity ($C_i$), as expressed in Eq. (3). Similarly, the amount of product that can be processed ($x^{product}_{i,j}$) by plants B, C, and M is limited by the capacity of each processing plant, as expressed in Eq. (4). The capacity of plant D is constrained by the amount of product supplied from plants C and M, as expressed in Eq. (5). $W^{EG}$ and $W^{PTA}$ are the weight fractions of products from plant C and Plant M, respectively. Finally, Eq. (6) refers to the mass flow limitation of product from plant D to Demand. A minimum capacity constraint was included to force the model to select feedstock suppliers and intermediate processing plants that can supply enough biomass and products to supply (at least) 80% of the demand, as shown in Eq. (7).

$$\sum_{j\in Pd} x^{product}_{i,j} \geq C_i * 0.8 \qquad \forall\ i \in D \tag{7}$$

*Mass balance*

$$\sum_{m\in M}\sum_{r\in R} x^{b}_{m,r,i} * Y^{b}_{m,i} = \sum_{j\in Pb} x^{product}_{i,j} \tag{8}$$

$$\sum_{j\in Pa} x^{product}_{i,j} * Y^{product}_{i} = \sum_{j\in Pc} x^{product}_{i,j} \tag{9}$$

$$\sum_{j\in Pb} x^{product}_{i,j} * Y^{product}_{i} = \sum_{j\in Pd} x^{product}_{i,j} \qquad \forall\ i \in P_C \tag{10}$$

$$\sum_{j\in Pc} x^{product}_{i,j} * W^{EG} + \sum_{j\in Pm} x^{product}_{i,j} * W^{PTA} = \sum_{i\in D} x^{product}_{i,j} \tag{11}$$

**Equations (8 – 11)** represent the mass balance of each supplier $r$ and entity $i, j$ in the supply chain network. Eq. (8) describes the conversion of feedstock $m$ in plant A, where $Y^{b}_{m,i}$ is the conversion yield of feedstock $m$ in plant $i$. Similarly, the conversion of intermediate products in plants B and C is expressed in Eqs. (9 and 10), where $Y^{product}_{i}$ is the conversion yield of product in each processing plant. Eq. (11) represents the mass balance in Plant D to supply the demand D.

*Operational constraints*

$$\sum_{i\in I}\sum_{n\in N} up_{i,n} \leq Np \tag{12}$$

Eq. (12) assures that the number of selected plants is lower or equal to the number of available plants ($Np$).

### 2.1.4. Cost assessment

The objective function that describes the economic costs of the supply chain was divided into six terms, as shown in Eq. (13). The first term (***A***) concerns the feedstock supply costs, including feedstock production costs (at farm level) and the transportation costs from region $r$ to plant A. The second term (***B***) expresses the capital and operative costs of plant A controlled by the binary variable $up_{i,n}$, which is equal to 1 when entity $i$ and plant size $n$ are open. Similarly, the third term (***C***) presents the capital and operative costs of plants B, C, M and D. The fourth term (***D***) expresses the transportation costs on intermediate products between the different entities (plants B, C, M, D). Finally, term (***E***) expresses the profits for selling the co-products $g$ of plant A in the market.

$$Prod.\ Costs = \sum_{m\in M}\sum_{r\in R}\sum_{i\in Pa} x^{b}_{m,r,i} * \left[ B^{cost}_{m,r} + \sum_{s\in S}\left(T^{fix}_{r,s} + T^{var}_{r,s}\right) * Z_{r,i,s} \right] (\boldsymbol{A})$$

$$+ \sum_{m\in M}\sum_{i\in Pa}\sum_{n\in PaSz}\left(CAP_{m,i,n} + OP^{fix}_{m,i,n} + OP^{var}_{m,i,n}\right) * up_{i,n} (\boldsymbol{B})$$

$$+ \sum_{i\in I}\sum_{n\in N}\left(CAP_{i,n} + OP^{fix}_{i,n} + OP^{var}_{i,n}\right) * up_{i,n}\ (\boldsymbol{C})$$

$$+ \sum_{i\in I}\sum_{j\in J}\left( x^{product}_{i,j} * \sum_{s\in S}\left(T^{fix}_{i,s} + T^{var}_{i,s}\right) * Z_{i,j,s} \right) (\boldsymbol{D})$$

$$- \sum_{m\in M}\sum_{g\in G}\sum_{i\in Pa} x^{co-prod}_{g,i} \$^{co-prod}_{m,g,i}\ \ (\boldsymbol{E}) \tag{13}$$

*2.1.5. Environmental assessment*

The objective function that describes the environmental costs of the supply chain includes the GHG emissions from transportation ($T^{emi}$) and GHG emissions of the process ($P^{emi}$) converted to monetary values by using carbon taxation, as expressed in **Eq. (14)**.

$$Env.\ Costs = \left[T^{emi} + P^{emi}\right]\$^{carbon\ tax} \tag{14}$$

The transportation emissions were calculated as the product of the mass flow exchanges and the transportation distances between different suppliers and entities, as expressed in **Eq. (15)**. Emission factors ($E_s$) of the transportation modes (truck and train) were obtained from Ecoinvent V3.4 database.

$$T^{emi} = \sum_{s\in S}\sum_{m\in M}\sum_{r\in R}\sum_{i\in Pa} x^{b}_{m,r,i} * Z_{r,i,s} * E_s + \sum_{s\in S} + \sum_{s\in S}\sum_{g\in G}\sum_{i\in I} x^{co-prod}_{g,i} * E_s * Z^{co-prod} \tag{15}$$

The process emissions were calculated as the product between the final product mass flow and the GHG emissions ($E_{m,i}$) from its production, as expressed in **Eq. (16)**. LCA tool was used to calculate the GHG emissions of the cradle-to-gate production process. The results from the LCA were obtained from a previous study (Garcia-Velasquez and van der Meer, 2021). The carbon tax was selected as the carbon-pricing policy to add a monetary value to the GHG emissions.

$$P^{emi} = \sum_{m\in M}\sum_{i\in Pd}\sum_{j\in D} x^{product}_{i,j} * E_{m,i} \tag{16}$$

*2.1.6. Single-objective approach*

A single objective approach was used to account for the environmental impacts on the economic costs of the supply chain, aiming to minimize the total costs, as shown in **Eq. (17)**. The *BeWhere* model comprises interfaces between different software modalities such as Excel, Python, and GAMS (General Algebraic Modeling System). We used excel to collect data on the different parameters (as described in the nomenclature list). GAMS was used to perform the optimization of the objective function. Besides, Python was utilized as an interface between Excel and GAMS. Data from Excel files were converted into text files that are input to the optimization model in GAMS. We created a GitHub repository (https://github.com/caaficus/BeWhere-model) where the excel dataset, python files, and GAMS code are available.

$$\min Total\ Costs = Prod.\ Costs + Env.\ Costs \tag{17}$$

*2.2. Case study*

Polyethylene Terephthalate (PET) is one of the most consumed thermoplastic polymers worldwide. The European demand for PET was approximately 4 million tons in 2018, and it is expected to increase due to the need for plastic bottles for soft drinks (PlasticsEurope, 2019). Most PET is produced from fossil-based sources, making the process highly profitable (due to the current low oil prices). The production of PET polymer involves two monomers at different ratios: mono ethylene glycol (MEG) that comprises 30% by weight of the final PET polymer, and purified terephthalic acid (PTA) that contributes to 70% by weight. These monomers are produced from the cracking of naphtha (MEG) and steam reforming of natural gas (PTA). However, the increasing awareness of the negative environmental impacts of fossil-based resources has boosted the development of alternative solutions for PET production using renewable resources. The Coca-Cola Company made the first approach in 2009 when the first partially biobased PET bottle under the label "PlantBottle" was introduced (Anderson, 2015). “PlantBottle” has a 30% biobased content due to the use of MEG from sugarcane ethanol as a substitute for the naphtha MEG, while the PTA is still fossil-based. The 30% biobased PET bottle production still depends on crude oil for the PTA production and the supply chain of MEG depends on the ethanol production from sugarcane in Brazil and India (global supply chains) (Knutzen, 2016). Biobased PTA production has emerged as an alternative aiming to produce 100% biobased PET. However, due to its high production costs (compared to fossil-based) (Athaley et al., 2019) and high GHG emissions (Volanti et al., 2019), it is not attractive for stakeholders. In previous work (Garcia-Velasquez and van der Meer, 2021), the production of biobased PTA combined with the development of local supply chains (mainly sugar beet) evidenced better environmental impacts than the traditional supply chains. Therefore, this paper aims to gather the previous knowledge from the environmental assessment of biobased PET and integrate it into the design of local supply chain networks for biobased PET production using locally available biomass, such as sugar beet (for MEG and PTA production) and wheat (for MEG production). A schematic description of the supply chain network for the biobased PET production is presented in Fig. 2. The biobased MEG production involves different entities from the feedstock supplier $R$, ethanol production $P_A$, ethylene production $P_B$ and ethylene oxide/ethylene glycol (EO/EG) production $P_C$. The production of PTA comprises two pathways: fossil-based and bio-based, using sugar beet as feedstock. The production of both fossil-based and biobased PTA occurs in the same location $P_M$ since there are no available production plants of biobased PTA in Europe. Both biobased MEG and fossil/biobased PTA are transported to the PET production $P_D$, and then the PET polymer is transferred to the demand $D$, where pre-form PET bottles are produced.

*2.3. Spatial distribution of sugar beet and wheat in Europe*

One of the main constraints for developing a biobased supply chain is feedstock availability, as introduced in **Eq. (2)**. Data for $B^{avail}_{m,r}$ were collected from the Global Biosphere Management Model (GLOBIOM) developed in the International Institute of Applied Systems Analysis (IIASA) (Havlík et al., 2011). The database contains information about the total production, distribution among different uses (e.g., feed, food, others), imports, and exports for several feedstocks (including sugar beet and wheat) in EU countries. The data are categorized among EU countries using the Nomenclature of Units for Territorial Statistics (NUTS). Arc-GIS software was used to determine the feedstock supply location in the EU using a NUTS-2 distribution, as presented in Fig. 3.

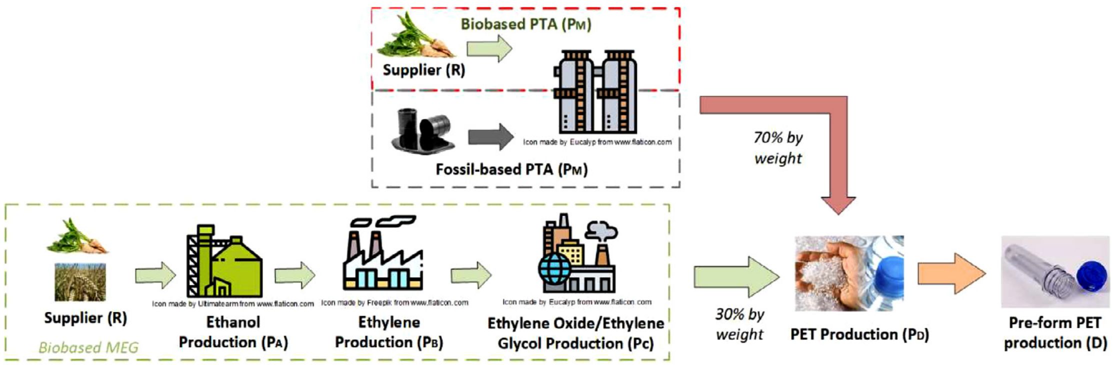


**Fig. 2.** Schematic description of the production of both 30% and 100% biobased PET using sugar beet and wheat as raw materials.

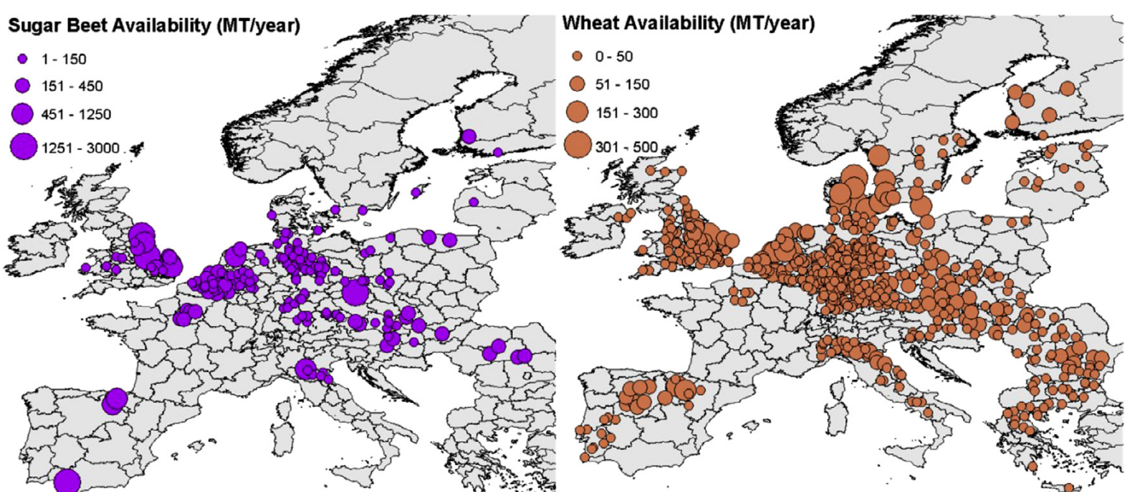


**Fig. 3.** Spatial location of the available biomass (sugar beet and wheat) in Europe.

### 2.4. Entities location

The geographical location and capacity of the different entities involved in the biobased supply chain were collected from different sources, such as NGOs (non-governmental organizations), industrial parks', and companies' websites. Information about the ethanol plants was obtained from the European Renewable Ethanol (ePURE) website (European Renewable Ethanol (ePURE), 2020). Information regarding ethylene, EO/EG, PTA, and PET plants were directly collected from companies' websites. This information was processed and displayed as a Google map (Garcia-Velasquez, 2021). The map has eight layers containing information about the feedstock suppliers (NUTS-3 identification, geographical location, and available biomass), ethanol plants (processed feedstock, country, company's name, and ethanol capacity), ethylene, EG, PTA, and PET plants (same information as for the ethanol plants). The demand for PET to produce pre-form PET bottles was distributed among EU countries. The design of the biobased supply chain assumes to supply a demand of 1.8 million tons per year of PET, which represents 45% of the total converters demand in Europe in 2019 (PlasticsEurope, 2019).

### 2.5. Life cycle assessment (LCA)

The environmental impact of the production of 1 kilogram of bottle-grade biobased PET at factory-gate using different feedstocks was obtained from previous work (Garcia-Velasquez and van der Meer, 2021). The use of biomass to produce chemicals might mitigate certain environmental impacts of fossil-based chemicals. Fig. 4 summarizes the results from the GHG emissions from fossil-based PET and bottle-grade biobased PET from sugar beet and wheat, including biogenic emissions and land use change (LUC) emissions. Biogenic emissions were included as a deduction to the total GHG emissions for the cradle-to-gate production of bottle-grade biobased PET, as suggested by (Pawelzik et al., 2013). The contribution of each entity (e.g., ethanol, ethylene, PTA, etc.) to the GHG emissions of the 30% and 100% biobased production is represented in Fig. 5, where PTA production contributes to most of the GHG emissions.

However, PET plants are located in different countries, and therefore the environmental impacts of producing PET in each country differ from one to the other (e.g., energy matrices). Table 1 presents the results from the influence of the heat source and electricity matrix of different EU countries on the total GHG emissions (including biogenic and LUC change).

Besides the process emissions, the optimization model considers the emissions from transportation from different transportation modes and distances. The distance between the feedstock suppliers and the different entities was estimated from the EU transportation network, including roads for trucks and railways for trains. ArcGIS extension – Origin-Destination cost matrix analysis was used to determine the shortest route between the multiple entities. Additionally, emission factors of the transportation modes (truck and train) were obtained from Ecoinvent V3.4, as summarized in Table 2.

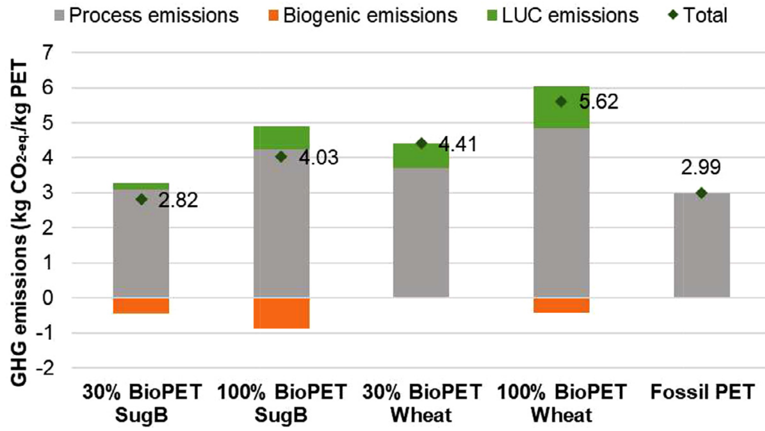


**Fig. 4.** Comparison of GHG emissions from fossil PET and bottle-grade biobased PET from sugar beet and wheat.

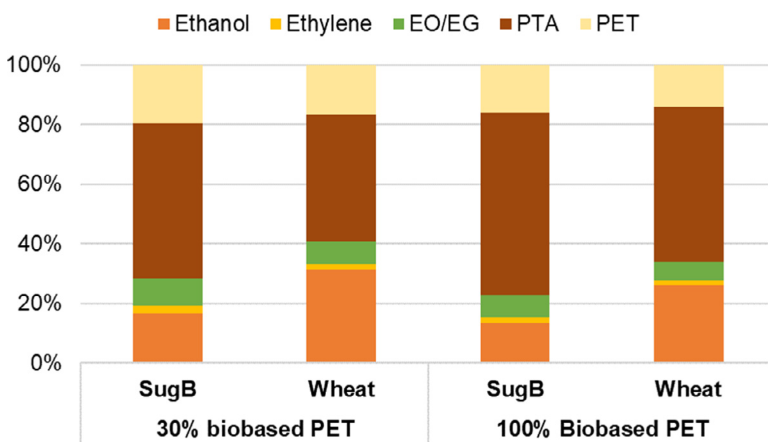


**Fig. 5.** Contribution of each entity to the GHG emissions of the 30% and 100% biobased PET production.

**Table 1**
GHG emissions (including biogenic and LUC emission) of 30% and 100% bottle-grade biobased PET from sugar beet and wheat.

| Countries | 30% BioPET (kg $CO_{2-eq.}$/kg PET) | | 100% BioPET (kg $CO_{2-eq.}$/kg PET) | |
|---|---|---|---|---|
| | Sugar Beet | Wheat | Sugar Beet | Wheat |
| Austria | 2.547 | 4.212 | −0.296 | 3.269 |
| Belgium | 2.447 | 4.146 | −0.317 | 3.170 |
| Czech Republic | 2.924 | 4.462 | −0.217 | 3.647 |
| Denmark | 2.668 | 4.293 | −0.271 | 3.391 |
| Estonia | 2.635 | 4.270 | −0.278 | 3.357 |
| France | 2.435 | 4.138 | −0.319 | 3.158 |
| Germany | 2.554 | 4.217 | −0.294 | 3.277 |
| Greece | 2.851 | 4.413 | −0.233 | 3.573 |
| Hungary | 2.649 | 4.280 | −0.275 | 3.372 |
| Lithuania | 2.469 | 4.161 | −0.312 | 3.192 |
| Netherlands | 2.668 | 4.293 | −0.271 | 3.391 |
| Poland | 3.185 | 4.635 | −0.163 | 3.908 |
| Slovakia | 2.835 | 4.403 | −0.236 | 3.558 |
| United Kingdom | 2.569 | 4.227 | −0.291 | 3.292 |

*2.6. Life cycle costing (LCC)*

LCC is the analysis of the costs (direct and indirect, variables, and fixed) assigned to a product/service starting from the contextualization of the idea until the end-of-life. Biomass costs (production and transportation), production costs (entities' production costs), and transportation costs between the different entities were included to keep the same system boundaries as the LCA. Biomass production costs were collected from the GLOBIOM database (Havlík et al., 2011) under a business-as-usual scenario for 2020 in the different EU countries, as summarized in the **Supplementary Material.** Biomass transportation costs were divided into fixed and variable costs. Fixed biomass transportation costs depend on the transportation mode, and these values were obtained from Ecoinvent v3.4, as shown in Table 3. The variable biomass transportation costs were estimated based on the fuel consumption per type of transportation (taken from Ecoinvent v3.4) and the diesel/electricity market price (European Commission, 2019) in each EU country.

The production costs of the different entities were categorized as capital and operating expenditures. Capital expenditures (CAPEX) are fixed expenses incurred on purchasing land, build-

**Table 2**
Emission factors of the transportation modes in the network analysis.

| Transportation Mode | Description | Emission Factors* |
|---|---|---|
| Truck | Truck 16 – 32 t with EURO 6 engine and diesel as fuel | 0.166 |
| Train | Train using diesel and electricity (Average EU countries) | 0.026 |

* Units - kg $CO_2$/tkm.

**Table 3**
Freight costs of the different transportation modes in the network analysis.

| Transp. Mode | Description | Fuel Consumption[1] | Freight Price[2] |
|---|---|---|---|
| Truck | Truck 16 – 32 t with EURO 6 engine and diesel as fuel | 0.0366 | 0.028 |
| Train | Train using diesel and electricity (Average EU countries) | Diesel - 0.00068 | |
| Electricity - 0.0478* | 0.026 | | |

[1] *Units - kg/tkm.* [2]*Units - €/tkm.* **Units – kWh/tkm.*

ings, construction, and equipment used to produce goods. CAPEX is the Total Investment Costs (TIC) in this paper. Secondary resources (published papers, reports) were used to collect information on different entities' TIC's costs. A detailed description of the TIC for each entity is presented in the **Supplementary Material**. TIC are adapted to 2020 using the Chemical Engineering Plant Cost Indexes (CEPCI) published monthly in the Chemical Engineering Magazine ("Chemical Engineering Plant Cost Index (CEPCI)," 2019). The investment costs were annualized based on the economic lifetime (20 years) of the project and the interest rate of each country using **Eq. (18)**.

$$AC = \frac{IR}{1 - 1/(1+IR)} \tag{18}$$

Where,

AC – Annualized Cost (€/year)TIC – Total Investment Costs (€)
IR – Interest Rate (%) (see **Supplementary Material**)
t – Economic life

The operating expenditures (OPEX) are those needed to operate the facility or equipment, such as raw material/reagents, utility, maintenance, and labor costs. Reagents and utility costs were calculated from the mass balance of the process (as reported in (Garcia-Velasquez and van der Meer, 2021) and the market price reported in different databases (e.g., ICIS Pricing) or using the data published by (Straathof and Bampouli, 2017) and (Ulrich and Vasudevan, 2006). Commodity prices were adjusted to 2020 using the Producer Price Index, as reported in (U.S. Bureau of Labor Statistics, 2020). Table 4 summarizes the main economic data of feedstocks, reagents, and utilities used to perform the LCC of biobased PET production. Extra costs such as labor, maintenance, general and administrative costs were estimated using factors reported in different reports and publications (Couper, 2003; Douglas, 1988; Peters and Timmerhaus, 1991). A summary of these extra costs is presented in the **Supplementary Material**.

### 2.7. Carbon-pricing policy

The carbon tax was selected as the carbon-pricing policy to account for the GHG emissions within the BeWhere model. A carbon tax is a relatively easy carbon-pricing policy to implement that promotes green investment (Waltho et al., 2019). However, the main challenge of the carbon tax is to establish a proper rate, which is why it varies from one country to another. Some countries do not even use a carbon tax as a carbon policy but other systems like the EU emission trading scheme (ETS) and carbon caps (World Bank, 2019). Due to the variability in the carbon tax prices, a sensitivity analysis was carried out to analyze the influence of the environmental costs on the production costs of the intermediate products (ethylene, EG, PTA) and the final product (biobased PET). Carbon tax prices from zero to 150 €/t $CO_2$ were selected. A zero value considers no carbon tax. A 25 €/t $CO_2$ is consistent with the average carbon tax reported for several EU countries (World Bank, 2019). Two intermediate carbon tax prices were selected 50 and 100 €/t $CO_2$, following the required carbon price to fulfill the Paris Agreement minimum temperature targets in 2020 and 2035, respectively (World Bank, 2019). Finally, a carbon tax of 150 €/t $CO_2$ was included to consider a future scenario where the social cost for GHG emissions is accounted for (Ricke et al., 2018).

## 3. Results

This section presents the main outcomes from the optimization model, starting with the distribution of the economic and environmental costs for the production of 30% and 100% biobased PET, followed by the influence of the transportation and processes emissions in the total environmental impact of the biobased supply chain. Afterward, the influence of the feedstock (sugar beet and wheat) and the carbon tax price is analyzed. The different intermediates/entities' contribution to the economic performance of biobased PET is assessed. Finally, one of the main outcomes of the model is developing a biobased supply chain network (as Google Map) to produce biobased PET in Europe.

### 3.1. Accounting for scope 3 GHG emissions in the BeWhere model

Table 5 summarizes the total costs of the biobased supply chain for 30% and 100% biobased PET production using sugar beet and wheat. The total economic costs of the supply chain are higher when using wheat than sugar beet as feedstock for biobased PET production. The production of 100% biobased PET resulted in almost double the economic costs of producing 30% biobased PET due to the extra costs for biomass to produce PTA and the extra transportation costs. However, there are no significant differences in the economic costs of producing, for example, 30% biobased PET using sugar beet or wheat.

On the other hand, the environmental costs of producing biobased PET using wheat are higher than those from sugar beet due to the higher GHG emissions from wheat-producing biobased PET. The environmental costs for producing 100% biobased PET are higher than those for 30% biobased PET with 24% and 17% for sugar beet and wheat, respectively. The biggest contributor to the total environmental costs are the process emissions, accounting for more than 90% of the total emissions of the biobased supply chain (see Table 6). The process emissions from the production of biobased PET using wheat were the highest due to the high GHG emissions compared to sugar beet. However, the transportation emissions were higher for the sugar beet supply chain due to the low conversion rate of sugar beet to ethanol (0.21 kg

**Table 4**
Market price/assumptions of the LCC model for biobased PET production.

| Parameter | Value | Unit | Reference |
|---|---|---|---|
| Sodium Hydroxide (50%) | 391.3 | €/t | (ICIS, 2006) |
| Sulfuric Acid | 41.9 | €/t | (ICIS, 2006) |
| Ammonia (27%) | 323.6 | €/t | (ICIS, 2006) |
| Coke | 100 | €/t | (ICIS, 2006) |
| Limestone | 50.3 | €/t | (ICIS, 2006) |
| Process Water | 0.326 | €/$m^3$ | (Ulrich and Vasudevan, 2006) |
| Ethanol | 464 | €/t | (Bloomberg, 2020) |
| Ethylene | 1174.6 | €/t | Average Price (Straathof and Bampouli, 2017) |
| EG | 1211.9 | €/t | Average Price (Straathof and Bampouli, 2017) |
| PTA | 764.4 | €/t | Average Price (Straathof and Bampouli, 2017) |
| PET | 1142 | €/t | Average Price (Straathof and Bampouli, 2017) |
| Sugar beet | Supplementary Material | | |
| Wheat | Supplementary Material | | |
| Sugar beet pulp | Supplementary Material | | |
| Distiller's dried grains with solubles (DDGS) | Supplementary Material | | |
| Natural Gas | Market Price per country (Eurostat, 2020a) | | |
| Electricity | Market Price per country (Eurostat, 2020b) | | |

**Table 5**
Total costs of the biobased supply chain for the 30% and 100% biobased PET production from sugar beet and wheat.

| Total Costs (million EUR) | 30% BioPET Sugar Beet | 100% BioPET Sugar Beet | 30% BioPET Wheat | 100% BioPET Wheat |
|---|---|---|---|---|
| Economic costs | 1629.9 | 3607.9 | 1674.8 | 3646.7 |
| Environmental costs | 114.4 | 142.3 | 178.9 | 209.8 |
| Total | 1744.3 | 3750.2 | 1853.7 | 3856.5 |

**Table 6**
Total supply chain emissions from the production of 30% and 100% biobased PET.

| SC emissions (t $CO_{2\text{-eq.}}$) | 30% BioPET Sugar Beet | 100% BioPET Sugar Beet | 30% BioPET Wheat | 100% BioPET Wheat |
|---|---|---|---|---|
| Transportation | 138.7 | 238.8 | 40.3 | 121.4 |
| Process | 4436.1 | 5452.7 | 7115.7 | 8272.0 |

ethanol/kg sugar beet (Althoff et al., 2013)) compared to wheat (0.29 kg ethanol/kg wheat (Rosenberger et al., 2002)). Additionally, the wide availability of wheat in the EU (mostly concentrated in Germany, the Netherlands, Belgium, and the UK) will reduce the transportation distances between the wheat feedstock supplier and the bioethanol plants.

### 3.2. Influence of the feedstock selection and carbon tax in the feasibility of biobased PET

The production costs of both biobased PET using sugar beet and wheat were evaluated under different carbon tax prices to better understand the influence of the environmental costs on the total supply chain costs of the 30% and 100% biobased PET, as shown in Fig. 6. The production costs of the biobased and fossil-based PET increased with the carbon tax value. The influence of the carbon tax on the production costs of biobased PET was stronger when wheat was used as feedstock (higher value of *m*) due to the high GHG emissions compared to the use of sugar beet (see, Fig. 4). The 30% biobased PET production had the lowest influence (lowest value of *m*). The 100% biobased PET resulted in higher production costs (using wheat-based or sugar-based MEG and sugar-based PTA) than the fossil PET. Lower production costs were determined for the 30% biobased PET for carbon tax values below 100 €/t $CO_2$. However, a different behavior was evidenced for carbon tax values above 100 €/t $CO_2$, where the production of 30% biobased PET from wheat surpassed the price of fossil PET.

An in-depth analysis of the influence of the costs of intermediates in the total production costs of 100% biobased PET, using both feedstocks, revealed that PTA contributes to more than 60% of the production costs in the scenario with no carbon tax (see, Fig. 7), followed by the ethanol-ethylene-EO/EG pathways (accounting for less than 30% of the production costs), and the PET processing (10%). When the highest carbon tax value was taken, the environmental costs accounted for 28% and 38% of the total production costs using sugar beet and wheat, respectively. From the processing point of view, the PTA production costs remained the highest contributor, accounting for 45% for sugar beet biobased PET and 37% for wheat biobased PET. The same trend is evidenced for the 30% biobased PET (see **Supplementary Material**). Since the production of PET requires 70% PTA by weight, the production of this monomer is a crucial element in the economic profitability of biobased PET.

### 3.3. Comparison of intermediate production costs for biobased PET

From the economic assessment, the production costs of intermediates for biobased PET (e.g., EG and PTA) could be estimated. Table 7 presents the comparison of the production costs between the biobased intermediates and their market price. The main result

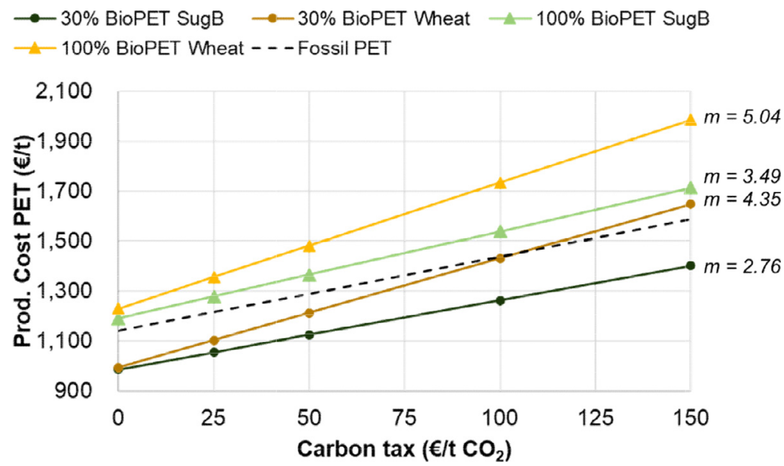


**Fig. 6.** Production costs of 30% and 100% biobased PET using sugar beet (SugB) and wheat as feedstock. *Slope (m) value represents the strong or weak influence of the carbon tax.*

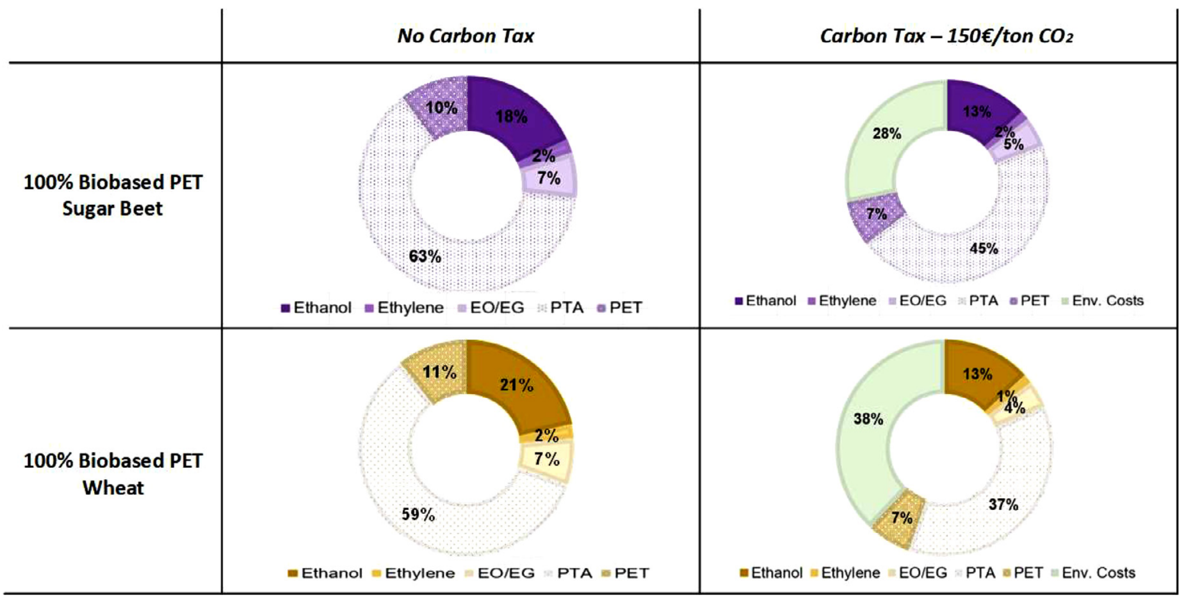


**Fig. 7.** Economic contribution of different intermediates in the total production costs of 100% biobased PET and the influence of feedstock and carbon tax.

**Table 7**
Comparison of production costs among intermediate products for producing biobased PET.

| Product | Units | Biobased | Market price[a] | %Change |
|---|---|---|---|---|
| EG – Sugar beet | EUR/t | 1174 | 1212 | −3.1% |
| EG - Wheat | EUR/t | 1265 | 1212 | 4.4% |
| PTA | EUR/t | 1057 | 764 | 38.4% |

[a] Market values are taken from (Straathof and Bampouli, 2017).

is that the production of biobased PTA (using sugar beet as feedstock) is unfeasible, with an increment of 38.4% compared to the fossil-based alternative. On the other hand, the production costs of EG from sugar beet and wheat evidenced opposed results. The production costs of biobased EG from sugar beet showed a reduction of 3.1% compared to the market price, whereas the use of wheat for biobased EG showed an increment of 4.4% in the production costs compared to the market price.

### *3.4. Design of the biobased supply chain network for the production of 30% biobased PET using sugar beet*

The supply chain network for the 30% biobased production using sugar beet was selected as an example of the data/information that the proposed tool can provide to the users as a Google Map (see Fig. 8 for a brief explanation of the features in the Google Map) (García-Velásquez, 2021). The selection of the displayed supply chain was made based on the economic and environmental results presented in the previous sections.

The map represents the supply chain logistics starting on the supply of sugar beet through the production of intermediate products (e.g., ethanol, ethylene) until the production of PET and its distribution to pre-form PET facilities (as the demand). The initial layout shows the distribution of multiple facilities for biomass, ethanol, and other products. Each icon represents an entity (e.g., biomass supply, entities locations). By clicking on the icons, the user finds information on the geographical location, economic parameters (CAPEX and OPEX), material flows, and production costs. A schematic representation of the transportation routes between the different entities was also included.

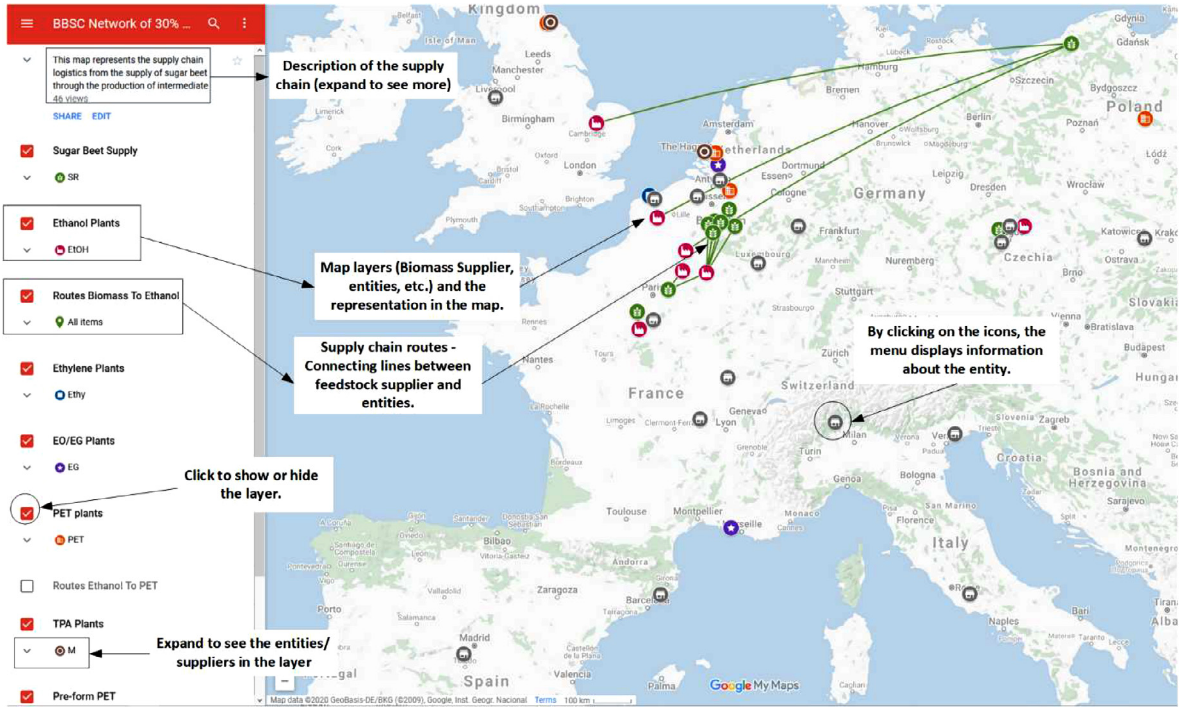


**Fig. 8.** Screenshot of the supply chain network for 30% biobased PET using sugar beet in Google Maps.

**Table 8**
Comparison of the contribution of the production and environmental costs to the total supply chain costs.

| References | Scenario | Productions costs (%) | GHG emission costs (%) |
|---|---|---|---|
| This work[a] | 30% Biobased PET – Sugar Beet | 93 | 7 |
| | 100% Biobased PET – Sugar Beet | 96 | 4 |
| | 30% Biobased PET – Wheat | 90 | 10 |
| | 100% Biobased PET – Wheat | 95 | 5 |
| (Chaabane et al., 2012) | Scenario 1[b] | 93.7 | 6.3 |
| | Scenario 2[c] | 93 | 7 |
| (Gerber et al., 2013) | Scenario 1[d] | 89 | 11 |
| | Scenario 2[e] | 92 | 8 |

[a] Carbon price = 25 €/t $CO_2$.
[b] Carbon price is stable at a value of 20 €/t $CO_2$.
[c] Carbon price increase over time starting at 2.5 to 20 €/t $CO_2$.
[d] Only electricity is produced from different sources (wood, geothermal, natural gas), and a carbon price of 60 €/t $CO_2$ was used.
[e] Heat and Power is produced from different sources (wood, geothermal, natural gas), and a carbon price of 60 €/t $CO_2$ was used.

## 4. Discussion

So far, only a few publications have evaluated the design of the supply chain accounting for external costs (e.g., environmental costs) in the economic profitability of a process. Most of these studies focused on GHG emissions from transportation and the manufacturing process (LCA emissions) (Chaabane et al., 2012; Gerber et al., 2013). From these studies, the carbon tax was the most used carbon-pricing policy to account for GHG emissions in the optimization models for designing biomass supply chains. However, the GHG emission costs did not strongly influence the total supply chain costs as presented in Table 8. The production costs account for more than 90% of the total supply chain costs, whereas less than 10% is attributed to the GHG emission costs. There is no significant influence of the carbon price (this work used 25 €/t $CO_2$ whereas other authors used higher values, such as 60 €/t $CO_2$). Therefore, the accounting of GHG emissions (from transportation and process) is not a strong criterion (alone) to play a key role in the design of biobased supply chains. The production of biobased PET also contributes to other impact categories (e.g., acidification, land use, eutrophication) (Chen et al., 2016; Garcia-Velasquez and van der Meer, 2021; Gomes et al., 2019). These 'externalities' should also be accounted for in economic terms in the optimization model to provide a full picture of environmental costs. However, the methodologies used to estimate these environmental prices differ from one model to another, providing different values for similar impact categories (Nguyen et al., 2016). Despite the uncertainty in the environmental prices, it is still a valid approach to quantify environmental impacts into monetary values.

Despite the fact that the GHG emission costs did not strongly influence the design of the biobased supply chains, they influenced the production costs per kilogram of biobased PET. Different parameters were identified to play a key role in the profitability of biobased PET: i) the selection of the feedstock (sugar beet vs wheat for MEG production), ii) the carbon tax price, and iii) the production costs of biobased PTA (for 100% biobased PET production).

There are currently no available publications (to our knowledge) on the economic assessment of the biobased PET production (or

MEG production) using sugar beet or wheat. However, bio-ethylene (the intermediate for MEG production) is an important platform molecule for the transition to a biobased economy, and information is available on the profitability of bio-ethylene using different feedstocks. According to (Mohsenzadeh et al., 2017), the production cost of bio-ethylene was 1200 and 2600 US$/t using sugarcane and sugar beet, respectively. The importance of the feedstock selection is evidenced, where sugar beet bio-ethylene costs were more than double the sugarcane bio-ethylene costs. In this study, a slight difference in the production costs of MEG using sugar beet and wheat was observed, as presented in Table 7.

The influence of the carbon tax on the economic performance of biobased PET was evaluated using different carbon prices (0 to 150 €/t $CO_2$). High carbon taxes do not encourage 100% biobased PET production due to the high GHG emissions compared to fossil PET. In the case of the 30% biobased PET, two patterns were detected. First, the production of 30% biobased PET (using sugar beet as feedstock for MEG) was not influenced by the carbon tax value due to the lower GHG emissions than the fossil PET. Secondly, the production of 30% biobased PET (using wheat for MEG production) was negatively influenced by the carbon tax after a value of 100 €/t $CO_2$, due to the higher GHG emissions compared to fossil PET. Therefore, this study demonstrated how an increase in the carbon tax value might not benefit the economic performance of both 30% and 100% biobased PET when GHG emissions of the production process (LCA) are included. However, this study also highlights the need to account for environmental impacts (e.g., GHG emissions) in the production costs of fossil PET, which might present the "true value" of producing fossil PET, and therefore; it might benefit the profitability of 30% biobased PET using sugar beet for MEG production.

The results from the environmental and economic assessment showed that the PTA production has the highest influence on the total production costs of both 30% and 100% biobased PTA. Improving the environmental performance of the biobased PTA production may enhance the profitability of the PTA production based on the framework proposed in this work. The environmental performance of the biobased PTA production can be improved through (i) the use of higher shares of renewable energy sources for heating (spotted as the hotspot of the production of biobased PTA (Garcia-Velasquez and van der Meer, 2021)) and (ii) the development of different technologies for biobased PTA production, such as the biobased BTX (benzene-toluene-xylene) process.

In this study, a decision-support tool was developed to guide decision-makers at any level (industry or government). Environmental impacts (mostly GHG emissions) are accounted for in monetary terms to assess biobased alternatives for plastics production. The tool is not limited to one application/product and thus can be used in various applications, including biofuels and other biochemicals. For the economic assessment, information about the CAPEX and OPEX of the processes included in the selected case is required to estimate the production costs. GHG emissions were selected as an environmental criterion due to their importance in the current transition to a climate-neutral economy. However, it is possible to include other impact categories such as eutrophication, human toxicity, and biodiversity loss through different monetization approaches. Assumptions and uncertainties of the selected monetization method should be considered, as already referred to in this section. Two feedstocks (sugar beet and wheat) were considered for their significant importance in developing EU agriculture. Sugar beet was selected as the most promising feedstock for the production of biobased PET. However, the tool allows using other types of agricultural products or lignocellulosic material, requiring data about the location of biomass suppliers, biomass trades (import and exports), and the current use of the biomass (food, feed, bioethanol).

## 5. Conclusion

The results from the decision-support tool highlight the importance of accounting for environmental impacts (GHG emissions from the process and transportation) in monetary terms for the design of supply chains for the production of biobased materials under the Paris Agreement and future climate policies. The design of biobased supply chains has relied on accounting for GHG emissions from transportation and not considering process emissions. In this work, process emissions accounted for more than 90% of the total supply chain emissions. However, environmental costs (only accounting for GHG emissions) had a low contribution to the total supply chain costs mainly due to two factors: i) exclusion of other impact categories (e.g., acidification, fossil depletion, eutrophication), and ii) the environmental accounting method (monetization, trade-offs). Including different environmental impacts and selecting the proper accounting method might help to boost the importance of environmental criteria in the design of biobased supply chains.

The design of supply chains for the 100% biobased PET production is not profitable due to the high economic and environmental contribution of the biobased PTA production. Biobased PTA was produced from sugar beet and accounted for up to 60% of the total GHG emissions from the process. Neither the use of sugar beet or wheat for MEG production positively affected the total supply chain costs of the 100% biobased PET. Therefore, different feedstocks (e.g., lignocellulosic biomass) and different technologies (e.g., fast pyrolysis) could be considered for biobased PTA production, aiming to mitigate the environmental impact compared to the current biochemical conversion of sugar beet. On the other hand, the feedstock selection significantly influenced the profitability of the 30% biobased PET. The 30% biobased PET using sugar beet (for MEG production) evidenced a better economic performance due to the low production costs and GHG emissions compared to the fossil PET. The use of wheat showed a good economic performance for carbon tax values below 100 €/t $CO_2$, due to higher GHG emissions than the fossil PET.

The optimization model was developed to provide insights on the importance of accounting for the environmental impacts of the production process. The optimization model promotes the conversation about the accounting of externalities (e.g., global warming potential, acidification, eutrophication) in the supply chain design together with the proper selection of accounting methods, either monetization or creating trade-offs between economic and environmental criteria (multicriteria). The model can be used for different applications (especially, the biobased chemical sector) and the selection of different feedstocks (agricultural products and lignocellulosic biomass). Basic knowledge of the supply chain of the biobased chemical product (supplier locations, plant locations, transportation network), economic parameters (CAPEX and OPEX), and environmental parameters (environmental impacts of transportation and process) are required for the model to select the most suitable configuration of biobased supply chains.

## 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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## Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.spc.2022.01.003.

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