USE OF OPTIMIZATION TOOLS FOR DECISION-MAKING: ACCOUNTING FOR EXTERNALITIES IN THE PRODUCTION OF BIOBASED PLASTICS

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ABSTRACT: Plastic is one of the most versatile materials, but its production relies on fossil-based resources that have been linked to the increase in GHG emissions. In this sense, biobased plastics arise as an alternative to completely or partly substitute these fossil-based plastics. Nevertheless, it is still unclear if the use of biomass for the production of bioplastics can mitigate the environmental impact of fossil-based plastics and simultaneously provide economic benefits. The proper design of biomass supply chains plays an important role in the development of biobased plastics; however, economic criteria (e.g., maximization of revenues) is the most used parameter to optimize the supply chain, whereas environmental criteria are barely considered. For this purpose, we propose an optimization model that evaluates different supply chain configurations for the production of biobased polyethylene terephthalate (PET) using sugar beet and wheat. The optimization model accounts for the production costs and environmental costs through different methodologies, such as the Life Cycle Costing (LCC) and Life Cycle Assessment (LCA), respectively. We found that the production of biobased terephthalic acid (TPA) directly influences the economic profitability of 100% biobased PET. The selection of feedstock and carbon tax scenario play an important role in the development of biobased supply chains.
Keywords: Life Cycle Assessment (LCA), Supply Chain, Biopolymers, Decision Support, Sugar Beet

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. Food and nutrition remain a cornerstone of the EU policy, but allow for unlocking the potential of the bioeconomy in Europe at the same time [1]. The bioeconomy sector had a total turnover of € 2.3 trillion, where the manufacture of biobased chemicals and plastics accounted for € 177 billion [1]. The creation of jobs in the biobased chemicals and plastic sector increased in the same period (see Figure 3 in the report from EC [1]). Despite the many benefits of the European bioeconomy, some limitations still hinder the full implementation. If we take the example of the biobased chemicals and plastic sector, the success of this industry depends on the lobbying efforts of governmental agencies, looking for incentives or regulations for the production of biobased products. This is well described in the book published by Lewandowski et al., [2] where the authors showed the interconnections between actors involved in the governance of the bioeconomy. On the other hand, there is the discussion on the environmental benefits of biobased products in comparison to fossil-based ones. Biobased products perform better in terms of GHG emissions, but there are concerns that the use of biomass as feedstock for the production of these materials can generate issues related to water and land use, biodiversity loss, eutrophication, among others [3]. However, the biobased industry claims that the comparison between fossil and biobased products is not fair, since the oil industry has a high technology maturity and some environmental impacts are not considered within the boundaries of the product system (e.g., oil spills) [4]. Despite the bottlenecks, the EC encourages the creation of new value chains and greener, more cost-effective industrial processes to support the modernization and strengthening of the EU bioeconomy [1]. Therefore, we must provide decision-makers/governmental entities with tools to start acting towards the setting of domestic value chains that promote the creation of local jobs and to provide incentives to industries promoting the shift from fossil-based to biobased products.

The design of Biomass Supply Chains (BSC) 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 [5]. A supply chain (SC) is defined as a combination of processes aimed at fulfilling customer's requests including different entities from suppliers, transporters, manufacturers, distributors, among others [6]. However, the design of a SC is traditionally linked to meet the customer's demands at the minimum cost, but the concept has expanded over time by including other criteria, such as minimizing the environmental and social impact. According to Barbosa-Povoa et al., [6], the most studied criteria in the design of SC are economic and environmental; however, the social criterion is attracting attention through the Sustainable Development Goals (SDG). The most used metrics within the economic criteria are the Total Costs (TC), profits and Net Present Value (NPV), whereas the environmental criteria cover metrics such as carbon dioxide (CO_2) emissions assessed as carbon footprint and greenhouse gasses (GHG) emissions.

The first decision-making issue we have to tackle is which criteria we should include in the design of BSC. 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 BSC and its effect, not only on economic but also environmental aspects [7]. For this purpose, Operational research (OR) has emerged as a discipline that following the optimization paradigm, helps the decision-maker to select the key criteria that will influence the overall quality of the decisions [8]. Among the different OR methods, optimization is commonly used to address the design of SC 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 [5]. TC seems to be the most adequate metric to optimize, and maybe the most convenient; however, the emphasis has changed towards multiple criteria to establish trade-offs between different alternatives and their consequences [9]. The use of economic and environmental criteria has become very popular due to the possibility of generating a portfolio of possible solutions for decision-makers that could select the best option based on their needs [5], [5], [10]. However, decision-makers face a challenge when presented with multiple criteria choices for the selection of the best SC. On the one hand, it is not clear how to deal with trade-offs between the different criteria, since decisions are subjective to the motivations or drivers of the decision-maker to select one configuration over the other. On the other hand, our society is highly driven by economic incentives, and thus a product with higher production costs and better environmental performance is not going to be considered due to the low economic performance [11]. As put forward by Tarnet et al., [11], environmental impacts could be addressed using monetary valuation methods (MVM) that translate the non-monetary impacts on the environmental and societal dimension into monetary terms [11]–[13].

Other approaches consider the design of BSC using carbon-pricing policies to account for the environmental impact of certain product or process, as reviewed by Waltho et al., [14]. Different carbon-pricing policies are applied to set a price or trade system to reduce GHG emissions from products or processes. The most popular ones are carbon tax, carbon cap, trade-and-cap, and carbon offset [14]. According to Waltho et al., the carbon tax and cap seem to be the most effective systems for reducing GHG emissions, and especially the carbon tax provides an extra incentive to invest in green technology [14]. In this sense, the purpose of our study is to use carbon-pricing policies, specifically the carbon tax to price emissions based on a tax rate, to guide decision-makers in the selection of the SC configuration, accounting for GHG emissions from the transportation network and production process under the life cycle assessment (LCA).

Emissions from transportation are widely included in the design of BSC with different carbon-pricing policies, whereas emissions from the product life cycle have not been widely considered. According to Waltho et al., [14], the main reason why emissions from LCA are not popular within the design of BSC is the high data requirements to perform the assessment. Furthermore, the GHG protocol provides guidelines for different emissions that companies should report. Companies are asked to report direct GHG emissions (scope 1), which are directly linked to transportation. Companies are not asked to report emissions from the upstream and downstream processing (scope 3) related to the LCA. The main concern regarding scope 3 emissions is double accounting, which has led to the absence of a requirement to report those emissions into their inventories. However, the importance of accounting for scope 3 emissions has been stressed due to the high contribution (up to 80%) of these emissions to the overall GHG inventory [15]. In summary, we acknowledge the importance to include scope 3 emissions into the design of BSC to promote the transition to a low-carbon economy, as biobased products can mitigate the negative environmental impacts from fossil-based products [3].

Despite the importance of biobased products to reduce our dependency on fossil-based products, the design of BSC through optimization models has focused mostly on the production of biofuels and electricity from renewable resources (e.g., agriculture products and wastes) [16]. We found a review paper from Dessbesell et al., [17] where only 5% of the reviewed papers (3 of 59 papers) evaluated the production of biobased materials and chemicals. After this review study was published in 2017, there has been an increasing interest in the design of SC for the production of biobased materials. We found that most of the papers on the topic "biobased supply chain (BBSC)" focus on the design of SC using as single criterion the production costs [18]–[20], whereas few publications include the environmental dimension, as a multiple objective optimization model [21], [22]. Therefore, we see the potential in the design of SC for the production of biobased materials involving economic and environmental criteria, specifically using carbon-pricing policies to raise public awareness that economic development in the production of these materials is possible as we account for the environmental benefits in its production.

In this sense, this paper aims to develop an optimization model for the design of BBSC using carbon-pricing policies. As a study case, we selected the production of biobased PET (polyethylene terephthalate) made from sugar beet and wheat in Europe. We believe that the production of biobased polymers is one of the options to reduce our dependency on fossil-based polymers and thus, mitigating the climate impact of crude oil. We propose a single-objective optimization model that involves two criteria: total production costs and environmental costs. Our model correlates the availability of biomass and supply logistics with the demand for PET to design a cost-effective SC that accounts for the environmental benefits/drawbacks of the production of biobased PET based on our previous work [3]. The economic criterion involves the calculation of the production costs using the Life Cycle Costing (LCC) framework, while the environmental criterion accounts for GHG emissions from the Life Cycle Assessment (LCA) into monetary values using carbon-pricing policies (e.g., carbon tax).

2 MODEL CHARACTERIZATION

2.1. Problem definition

This paper aims to determine the supply chain network at a strategic-decision level for biobased PET using the *BeWhere* model. This model is a spatially-explicit mixed-integer linear program (MILP) widely used in optimization studies for bioenergy production [23]–[27]. 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 [3] and the costs for emitting/mitigating GHG emissions are included in the model using carbon-pricing policies (e.g., carbon tax).

The optimization model used in this study is as follows:

Given

- The availability of feedstock and the location of the suppliers
- Feedstock cost per supplier location
- A possible superstructure for the location of SC entities (e.g., processing plants)
- Investment costs
- Operative costs (e.g., reagents costs, utility costs, labor costs)
- Transportation distances between the SC 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 SC entity
- Market prices of products from SC entities
- GHG emissions factors from the LCA
- GHG emissions factors for the different transportation modes
- Carbon tax
- Demand location and volume

Determine
- The SC network
- The flow amounts between SC entities
- The product cost in the SC entities

So as to
- Minimize the global SC costs
- Determine the effect of GHG emissions in the SC cost

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

2.2. Model formulation

The SC involves a two-stage structure: Feedstock supplier and plant A, plant A and plant B, plant B and plant C, plant C and plant D, Plant M and plant D, plant D and demand, as presented in Figure 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, Pm the plant M and D the demand.

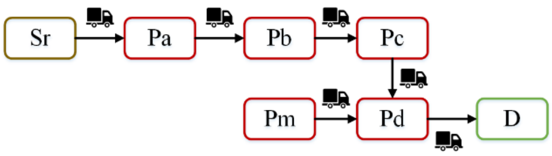

Figure 1: Schematic representation of the SC network.

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

2.2.1. Model constraints

In this section, we present the model constraints as characteristics that need to be guaranteed for the SC network design.

Feedstock availability

$$\sum_{m\in R_m}\sum_{r\in S_r}\sum_{i\in Pa} x^b_{m,r,i} \le \sum_{m\in R_m}\sum_{r\in S_r} B^{avail}_{m,r} \qquad (1)$$

Constraint (1) assures that the amount of feedstock m from region r to plant A is not higher than the amount of feedstock m available in region r. $B^{avail}_{m,r}$ is defined as the remaining amount of feedstock that can be potentially used for the production of biobased materials (see, Equation (2)), when the demand for food and feed has been supplied. We also included the feedstock trade (exports and imports) as an important factor that could increase or decrease the availability of biomass.

$$B^{avail}_{m,r} = B^{productivity}_{m,r} + B^{import}_{m,r} - B^{food}_{m,r} - B^{feed}_{m,r} - B^{export}_{m,r} \qquad (2)$$

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

$$\sum_{m\in R_m}\sum_{r\in S_r}\sum_{i\in Pa} x^b_{m,r,i} \le \sum_{i\in Pa}\sum_{n\in PaSz} c_i * UP_{i,n} \qquad (3)$$

$$\sum_{k\in P}\sum_{i\in I}\sum_{j\in I} x^P_{k,i,j} \le \sum_{i\in I}\sum_{n\in N} c_i * UP_{i,n} \qquad (4)$$

$$\sum_{k\in P}\sum_{i\in Pc}\sum_{j\in Pd} x^P_{k,i,j} * w_{EG} + \sum_{k\in P}\sum_{i\in Pm}\sum_{j\in Pd} x^P_{k,i,j} * w_{TPA} \le \sum_{i\in Pd}\sum_{n\in Pd} c_i * UP_{i,n} \qquad (5)$$

$$\sum_{k\in P}\sum_{i\in Pd}\sum_{j\in D} x^P_{k,i,j} \le \sum_{i\in D} c_i \qquad (6)$$

Constraints (3 – 6) describe the maximum amount of feedstock m or product k from one supplier/plant to another. Constraint (3) describes the amount of feedstock m that can be processed by plant A. Constraint (4) describes the amount of product k that can be processed by plants B, C and M. Constraint (5) describes the flow restriction from plant C and Plant M to plant D. Finally, constraint (6) describes the amount of product k in plant D to Demand. We also included a minimum capacity constraint to force the model to use the capacity of each plant above 80%, as shown in constraint (7).

$$\sum_{k\in P}\sum_{i\in I}\sum_{j\in I} x^P_{k,i,j} \ge \sum_{i\in I}\sum_{n\in N} c_i * UP_{i,n} * 0.8 \qquad (7)$$

Mass balance

$$\sum_{m\in R_m}\sum_{r\in S_r}\sum_{i\in Pa}\sum_{k\in P} x^b_{m,r,i} * eff^{Pa}_{m,i,k} = \sum_{k\in P}\sum_{i\in Pa}\sum_{j\in Pb} x^P_{k,i,j} \qquad (8)$$

$$\sum_{k\in P}\sum_{i\in I}\sum_{j\in I} x^P_{k,i,j} * eff^P_{i,k} = \sum_{k\in P}\sum_{i\in I}\sum_{j\in J} x^P_{k,i,j} \qquad (9)$$

$$\sum_{k\in P}\sum_{i\in Pc}\sum_{j\in Pd} x_{k,i,j}^{P} * w_{EG} + \sum_{k\in P}\sum_{i\in Pm}\sum_{j\in Pd} x_{k,i,j}^{P} * w_{TPA} = \sum_{k\in P}\sum_{i\in Pd}\sum_{j\in D} x_{k,i,j}^{P} \quad (10)$$

Equations (8 – 10) represent the mass balance of each supplier r and entity i, j in the SC network. Equation (8) describes the conversion of feedstock m to product k in plant A. Similarly, equation (9) describe the conversion of intermediate products in plant B and plant C Equation (10) represents the mass balance to produce product k in Plant D to supply demand D.

Operational constraints

$$\sum_{i\in I}\sum_{n\in N} UP_{i,n} \leq Np \quad (11)$$

Constraint (11) assures that the number of selected plants should be lower than the number of available plants (Np).

2.2.2. Cost assessment

We divided the objective function that describes the economic costs of the SC in six terms, as shown in equation (12). The first term (1) 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 (2) expresses the capital and operative costs of the plant A controlled by the binary variable $UP_{i,n}$ which equals 1 when entity i and plant size n are open. The third term (3) describes the transportation costs of product k from plant A to plant B depending on the feedstock m. The fourth term (4) discounts the profits for selling the co-products g of plant A in the market. The fifth and sixth terms $(5-6)$ represent the capital and operative costs, and the transportation costs of the intermediate products k in the intermediate entities (P_b, P_c, P_m), respectively.

$$\begin{aligned} Prod.Costs = {} & \textstyle\sum_{m\in R_m}\sum_{r\in S_r}\sum_{i\in Pa} x_{m,r,i}^{b} * \left[B_{m,r}^{cost} + \sum_{s\in T_s}\left(Tfix_{m,r,s}^{B} + Tvar_{m,r,s}^{B}\right) * Td_{m,r,i,s}^{B}\right] (\mathbf{1}) \\ & + \textstyle\sum_{m\in R_m}\sum_{i\in Pa}\sum_{n\in PaSz}\left(CAP_{m,i,n} + OP_{m,i,n}^{fix} + OP_{m,i,n}^{var}\right) * UP_{i,n} \ (\mathbf{2}) \\ & + \textstyle\sum_{k\in P}\sum_{i\in Pa}\sum_{j\in Pb}\left(x_{k,i,j}^{P} * \sum_{s\in T_s}\left(T_{i,s}^{fix} + T_{i,s}^{var}\right) * Td_{i,j,s}\right) (\mathbf{3}) \\ & - \textstyle\sum_{m\in R_m}\sum_{g\in CP}\sum_{i\in Pa} x_{g,i}^{CP} * CPP_{m,i,g} \ (\mathbf{4}) \\ & + \textstyle\sum_{i\in I}\sum_{n\in N}\left(CAP_{i,n} + OP_{i,n}^{fix} + OP_{i,n}^{var}\right) * UP_{i,n} \ (\mathbf{5}) \\ & + \textstyle\sum_{k\in P}\sum_{i\in I}\sum_{j\in I}\left(x_{k,i,j}^{P} * \sum_{s\in T_s}\left(T_{i,s}^{fix} + T_{i,s}^{var}\right) * Td_{i,j,s}\right) (\mathbf{6}) \end{aligned} \quad (12)$$

2.2.3. Environmental Assessment

The objective function that describes the environmental costs (Equation (15)) of the SC includes the emissions from the transportation (T_{emi}) and GHG emissions from LCA (P_{emi}) converted to monetary values using carbon-pricing policies. The transportation emissions were calculated as the product of the mass flow exchanges and the transportation distances between different entities, and emission factors as a function of the transportation mode (e.g., truck and train) (see, Equation (13)). The process emissions were calculated as the product between the mass flow of the final product and the process emissions from the Life Cycle Assessment (LCA) methodology (see, Equation (14)). We used data of a previous study for the process emissions of the SC [3]. We used carbon tax as the carbon-pricing policy to add a monetary value to the GHG emissions.

$$\begin{aligned} T_{emi} = {} & \sum_{s\in T_s}\sum_{m\in R_m}\sum_{r\in S_r}\sum_{i\in Pa} x_{m,r,i}^{b} * Td_{m,r,i,s}^{B} * e_s \\ & + \sum_{s\in T_s}\sum_{k\in P}\sum_{i\in I}\sum_{j\in I} x_{k,i,j}^{P} * Td_{i,j,s} * e_s \\ & + \sum_{s\in T_s}\sum_{g\in P}\sum_{i\in I} x_{g,i}^{CP} * Td_{CP} * e_s \end{aligned} \quad (13)$$

$$P_{emi} = \sum_{m\in R_m}\sum_{k\in P}\sum_{i\in Pd}\sum_{j\in D} x_{k,i,j}^{P} * e_{m,i} \quad (14)$$

$$Env.Costs = \left[T_{emi} + P_{emi}\right] * \$_{carbon\ tax} \quad (15)$$

2.2.4. Single-objective approach

Since the goal is to account for the environmental impacts in the economic costs of the SC, we decided to use a single objective approach where the main objective is to minimize the total costs, accounting for GHG emissions (in monetary values), as shown in Equation (16). The *BeWhere* model comprises interfaces between different software modalities such as Excel, Python, and GAMS (General Algebraic Modeling System). We used Excel to collect the information on the different parameters (see, appendix) and GAMS to perform the optimization of the objective function. We used Python as interface between Excel and GAMS, meaning that data from Excel files were converted into text files that are inputs to the optimization model in GAMS.

$$\min Total\ Costs = Prod.Costs + Env.Costs \quad (16)$$

3 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 of plastic bottles for soft drinks [28]. Most PET is produced from fossil-based sources, which makes 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 terephthalic acid (TPA) that contributes to 70% by weight. These monomers are produced from the cracking of naphtha (MEG) and steam reforming of natural gas (TPA). However, the increasing awareness of the negative environmental impacts of fossil-based resources has boosted the development of alternative solutions for the production of PET using renewable resources. The first approach was launched by the Coca-Cola company in 2009 when the first partially biobased PET bottle under the label "PlantBottle" was introduced [29]. "PlantBottle" has a 30% biobased content due to the use of MEG from sugarcane ethanol as a substitute for the naphtha MEG, while the TPA is still fossil-based. There are two main concerns with the 30% biobased PET bottle: first, it still depends on crude oil for the production of TPA and secondly, the SC of MEG depends on the production of ethanol from sugarcane in Brazil and India [30]. The technology to produce biobased TPA is at different development stages from demonstration to lab-scale; however, most of these technologies have been developed using corn as feedstock, adding to the food security debate [31]. In this sense, we propose the use of sugar beet for the production of biobased TPA, as an agricultural product that has been strongly hit by the low sugar prices in Europe and to promote policies that provide incentives to farmers for its production.

Global SCs have exposed their vulnerability amidst the COVID-19 pandemic, and thus local SC could provide supply security. We mean by local SC the complete network from the acquisition of feedstock until the final product to supply the internal demand for PET polymer within Europe. Therefore, we propose the design of local SC networks for the production of biobased PET using locally available biomass, such as sugar beet and wheat. A schematic description of the SC network for the production of biobased PET is presented in Figure 2. The biobased MEG production involves different entities from the feedstock supplier S_r, ethanol production P_A, ethylene production P_B and ethylene oxide/ethylene glycol (EO/EG) production P_C. The production of TPA comprises two pathways: fossil-based and bio-based using sugar beet as feedstock. We assume that the production of both fossil-based and biobased TPA takes place in the same location P_M since there are no available production plants of biobased TPA in Europe. Both biobased MEG and fossil/biobased TPA 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.

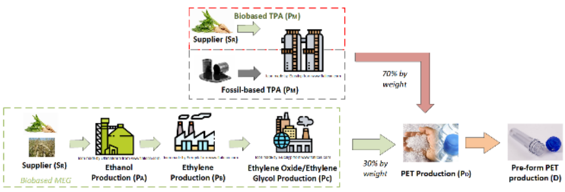

Figure 2: Schematic description of the production of both 30% and 100% biobased PET using sugar beet and wheat as raw materials.

3.1. Spatial Distribution of Sugar beet and Wheat in Europe

One of the main constrains for the development of a BBSC is the availability of feedstock, as introduced in Equation (2). We collected data for the calculation of $B_{m,r}^{avail}$ from the Global Biosphere Management Model (GLOBIOM) developed in the International Institute of Applied Science Analysis (IIASA) [32]. 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, using a business-as-usual reference model for the year 2020. The data are categorized among EU countries using the Nomenclature of Units for Territorial Statistics (NUTS-2). We used the software Arc-GIS to determine the location of the feedstock supply in EU using a NUTS-2 distribution, as presented in Figure 3.

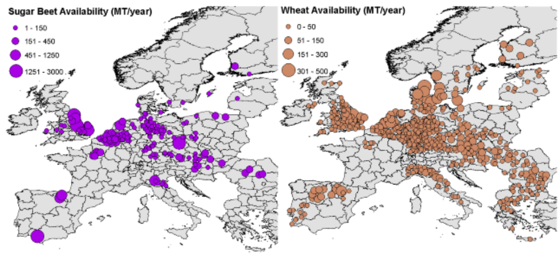

Figure 3: Spatial location of the available biomass (sugar beet and wheat) in Europe [32].

3.2. Entities Location

We collected information on the geographical location and capacity of the different entities involved in the BBSC using different sources, such as NGO (non-governmental organizations), industrial parks', and companies' websites. Information about the ethanol plants was obtained from the European Renewable Ethanol (ePURE) website [33]. Information regarding ethylene, EO/EG, TPA, and PET plants was directly collected from companies' websites. This information was collected and displayed as a Google map - https://bit.ly/2U7B7W1.

3.3. Life Cycle Assessment (LCA)

In this study, we took the LCA results from the paper by García-Velásquez and van der Meer [3], assessing the environmental impact of the production of 1 kilogram of bottle-grade biobased PET (bottle-grade) at factory-gate using different feedstocks. The methodology and the model assumptions are not includede here, but all avaialabe in reference [3]. Table I presents the results of the LCA of the production of biobased PET at the different entities and the comparison with the fossil-based counterpart. We assume that the production of biobased products can mitigate the negative impact of the use of fossil resources, and therefore we introduce an additional column *"Abatement"* in Table 1 that shows the difference between the GHG emissions of the biobased and fossil-based intermediates. Negative values mean a GHG credit (biobased is better than fossil) and positive values are GHG debits (fossil is better than biobased). Additionally, our optimization model considers different transportation modes and distances, and therefore we separately included the GHG emissions from the transportation between the different entities. For this purpose, we used the emission factors reported by Ecoinvent V3.4 as shown in Table II.

Table I: Comparison of fossil and biobased intermediate products for accounting GHG emissions into the *BeWhere* model.

Intermediate Product	Biobased*	Fossil*	Abatement*
Ethylene	0.72[a]	1.42	- 0.7[a]
	5.7[b]		4.28[b]
EG	0.81	0.95	- 0.14
TPA	2.63[c]	1.74	0.89

[*] Units - kg CO_{2-eq}/kg PET
[a] Using sugar beet ethanol
[b] Using wheat ethanol
[c] Sugar beet was used in the production of TPA.

Table II: Emission factors of different transportation modes.

Transportation Mode	Description	Emission Factors*
Truck	Lorry 16 – 32 tons with EURO 6 engine and Diesel as fuel	0.166
Train	Train using Diesel and/or Electricity (Average EU countries)	0.026

* Units - kg CO_2/tkm

3.4. Life Cycle Costing (LCC)

LCC is the analysis of the costs (direct and indirect, variables, and fixed) that can be assigned to a product/service starting from the contextualization of the idea until the end-of-life. To keep the same system boundaries as in the LCA, the costs related to the production of biobased PET included the biomass costs (production and transportation), production costs (plant production costs), and transportation costs between the different entities. The transportation logistic between the biomass supplier and entities was carried out using two different transportation modes: truck and train. The detailed information of the transportation modes was taken from Ecoinvent V3.4 and is presented in Table III.

Table III: Information on the transportation modes of biomass and intermediate products.

Transp. Mode	Description	Fuel Consumption[1]	Freight Price[2]
Truck	Lorry 16 – 32 tons with EURO 6 engine and Diesel as fuel	0.037	0.028
Train	Train using Diesel and/or Electricity (Average EU countries)	0.011	0.026

[1] Units - kg Fuel/tkm
[2] Units - €/tkm

Biomass production costs were collected from the GLOBIOM database [32] under a business-as-usual scenario in the year 2020 for the different EU countries. Biomass transportation costs were divided into two types of costs: fixed and variable costs. Fixed biomass transportation costs were taken from Ecoinvent v3.4 depending on the transportation mode (truck and train) and the functional unit was ton-kilometer (tkm). On the other hand, 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 [34] in each EU country.

The production costs of the different entities for the production of biobased PET were categorized as capital and operating expenditures. Capital expenditures (CAPEX) are fixed expenses incurred on the purchase of land, buildings, construction, and equipment used in the production of goods. In our study, CAPEX are named as Total Investment Costs (TIC) and we used secondary data (published papers, reports) to collect information on the different entities TIC's costs. TIC were adapted to 2020 using the Chemical Engineering Plant Cost Indexes (CEPCI) that are published in the Chemical Engineering Magazine monthly [35]. The investment costs were annualized based on the economic lifetime (20 years) and the interest rate of each country using Equation (17).

$$AC = \frac{IR}{1 - 1/(1+IR)^t} \cdot TIC \tag{17}$$

Where,
AC – Annualized Cost (€/year)
TIC – Total Investment Cost (€)
IR – Interest Rate (%)
t – Economic life

On the other hand, the operating expenditures (OPEX) are those needed for the operation of 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 and the market price reported in different databases (i.e. ICIS Pricing) or using the data published by Straathof et al., [36] and Ulrich and Vasideva [37]. Extra costs such as labor, maintenance, general and administrative costs were estimated using factors reported in different reports and publications [38]–[40]. A detailed description of the market price/assumptions used in the LCC are presented in Table IV.

Table IV: Market price/assumptions of the LCC model for bioPET production.

Parameter	Value	Unit	Reference
Sugar beet	61.24	€/ton	Average price (GLOBIOM)
Wheat	199.76	€/ton	Average price (GLOBIOM)
Sodium Hydroxide (50%)	391.3	€/ton	Market Price
Sulfuric Acid	41.9	€/ton	Market Price
Ammonia (27%)	323.6	€/ton	Market Price
Coke	100	€/ton	Market Price
Limestone	50.3	€/ton	Market Price
Process Water	0.326	€/cum	Market Price
Ethanol	464	€/ton	Market Price
Sugar beet pulp	23.3	€/ton	Market Price

Distiller's dried grains with solubles (DDGS)	46.4	€/ton	Market Price
Ethylene	1,174.6	€/ton	Average Price [36]
Ethylene Glycol	1,211.9	€/ton	Average Price [36]
Terephthalic Acid (TPA)	764.4	€/ton	Average Price [36]
PET	1,142	€/ton	Average Price [36]
Assumptions			
Parameter	**Value**	**Reference**	
Maintenance Costs	6% AC	Khatiwada et al., [24]	
General and Administration Costs	5% AC	Khatiwada et al., [24]	
Labor Costs	**Remark**		**Ref.**
Number Operators per Shift[a]	$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5}$		Turton et al., [41]

[a] Where N_{OL} is the # of operators per shift, P is the # of processing stages involving particulate solids and N_{np} is the # of other processing stages.

3.5. Carbon-pricing policy

The value attributed as a carbon tax varies from one country to another. Some countries do not even use carbon tax as carbon policy, but other systems, such as the EU emission trading scheme and carbon caps [42]. Due to the variability in the carbon tax value, we assessed different carbon tax values to analyze the influence of the environmental costs in the production costs of the intermediate products (ethylene, EG, TPA) and the final product (PET). We used five different values – 0, 25, 50, 100, and 150 €/ ton CO_2. The first value considers no carbon tax. The second value (€25/ ton CO_2) is consistent with the average carbon tax reported for several EU countries [42]. The third and fourth values considered a carbon tax of €50 and €100 per ton CO_2 that follows the required carbon price to fulfill the Paris Agreement minimum temperature targets in 2020 and 2035, respectively [42]. Finally, a carbon tax of €150/ton CO_2 was included to consider a prospective scenario where the social carbon cost for GHG emissions is accounted for [43].

4 RESULTS

4.1. Accounting for scope 3 GHG emissions in the BeWhere model

The shift from fossil-based to biobased resources to produce PET should provide economic benefits for stakeholders, and therefore we explored the production costs of both 30% and 100% biobased PET using sugar beet and wheat under different carbon tax values, as shown in Figure 4. The production costs of 30% biobased PET are lower than the 100% biobased PET and the PET market price. The production of 100% biobased PET using both feedstocks gives higher production costs than the market average price (€1,142/ton PET) for all carbon tax values. We found out that the high production costs of 100% biobased PET originates from the high costs to produce biobased TPA, as shown in Figure 5. Since the production of PET requires 70% by weight of TPA, the production of this monomer is a key element in the profitability of the biobased PET. The production costs of biobased TPA from sugar beet are far higher than the current market price (€764.4/ton TPA) with an increment ranging between 35% and 55% of the market price, depending on the carbon tax (see, Figure 5). The difference in the TPA production cost is related to the higher environmental impact of producing biobased TPA (see, Table 1).

The selection of feedstock makes a big difference in the production costs of both 30% and 100% biobased PET. Figures 6 and 7 present the production costs of the ethylene and MEG using wheat and sugar beet. The use of wheat for the production of both products increases the costs above the market price, while the use of sugar beet reduces the production costs due to the GHG credits from the production of ethylene and MEG using biomass sources (see, Table I).

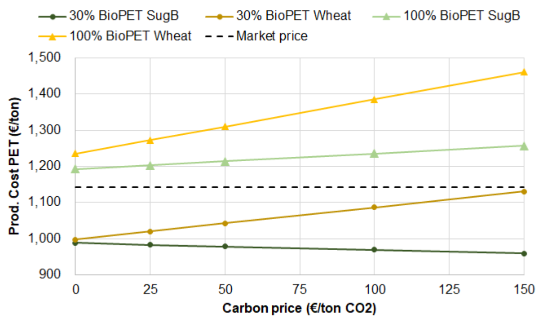

Figure 4: Production costs of 30% and 100% biobased PET using sugar beet (SugB) and wheat as feedstock.

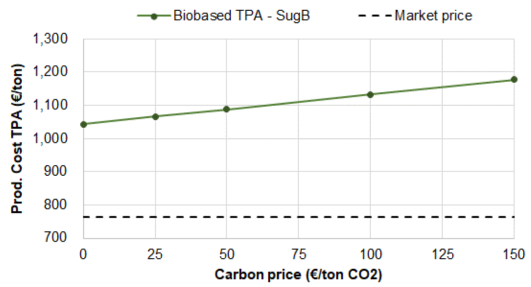

Figure 5: Production costs of biobased TPA using sugar beet (SugB).

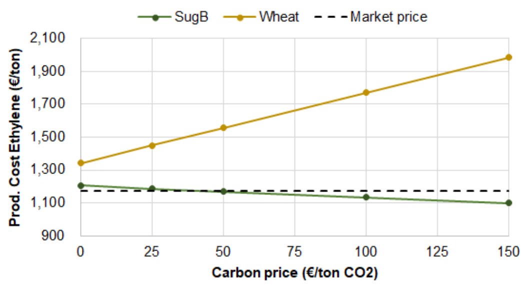

Figure 6: Production costs of ethylene using sugar beet (SugB) and wheat.

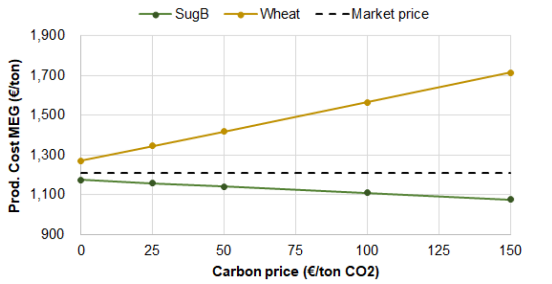

Figure 7: Production costs of MEG using sugar beet and wheat.

We calculated the profitability of the different entities at different locations to produce 30% biobased PET using both feedstocks, as summarized in Figure 8. We did not include the profitability assessment of the 100% biobased PET, since the production costs are higher than the market price, and therefore the profitability is negative throughout the 20 years of the project life. For both feedstocks, the production of 30% biobased PET in The Netherlands evidenced the highest profitability, but the payback period is also higher in comparison to other locations, like Greece. The difference lies in economic indicators per country, such as interest rate and inflation rates, where Greece has one of the lowest inflation rates (0.5%) in comparison to other locations, such as The Netherlands (2.7%).

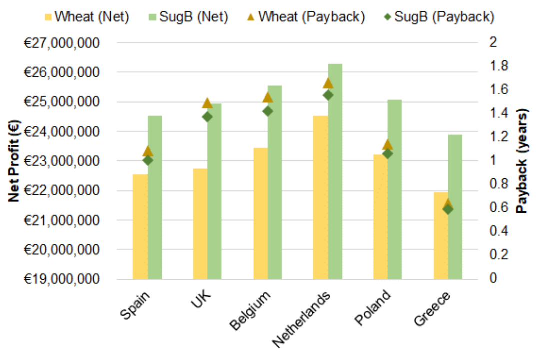

Figure 8: Net profitability and payback period of the production of 30% biobased PET. Bars represent the net profits (left) and points represent the payback period (right).

In the specific case of The Netherlands, the influence of carbon tax on the economic profitability of 30% biobased PET is strong when wheat is used as feedstock, as shown in Figure 9. Higher carbon tax values (up to 150 €/ton) can reduce the profitability to almost zero, while the payback period increases due to the low profits of the process. On the other hand, the net profits of the production of 30% biobased PET using sugar beet slightly increase, while the payback period remains almost unchanged.

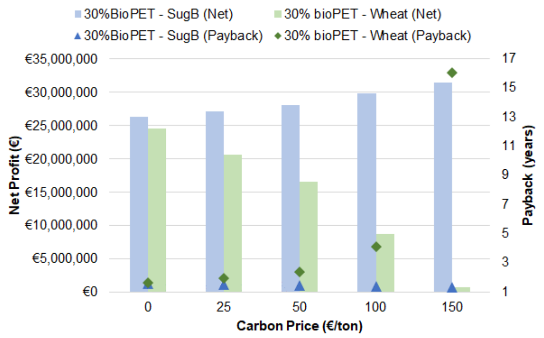

Figure 9: Effect of the carbon tax on the economic profitability of 30% biobased PET production using sugar beet and wheat.

5 CONCLUSION

The results from our optimization model highlight the importance of accounting for environmental impacts (GHG emissions) in the economic profitability of the production of biobased materials in view of the Paris Agreement and climate policies. The production of 100% biobased PET is not profitable due to the high economic and environmental contribution of the biobased TPA production. The use of biomass to produce biobased TPA increases the production costs of biobased PET but improves the environmental benefits of the biobased MEG production, depending on the feedstock. The use of biomass to produce biobased chemicals has also negative impacts to the environment. However, the environmental performance of the production of biobased TPA can be improved through (i) higher shares of renewable energy sources for heating, which was spotted as hotspot of the production of biobased TPA [3] and (ii) the development of different technologies for biobased TPA production, such as the biobased BTX (benzene-toluene-xylene) process. On the other hand, the production of 30% biobased PET showed good economic performance; the benefits are influenced by the feedstock selection and carbon tax values. The use of sugar beet to produce biobased MEG introduced a GHG credit when compared to the fossil-based pathway and thus, it provided economic benefits if a significant carbon tax is included.

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8 LOGO SPACE

9 APPENDIX: Model nomenclature

Indices

Consider the indices:

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

Sets

S_r as regions, $r \in S_r$
R_m as type of feedstock, $m \in R_m$
T_s as transportation mode, $s \in T_s$

Each level of the SC 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

Products and co-products

P as products in entities, $k \in P$
CP as co-products in entities, $g \in CP$

Parameters

Feedstock Supply

$B_{m,r}^{cost}$ unit cost of feedstock m in region r, $m \in R_m$ and $r \in S_r$
$B_{m,r}^{avail}$ availability of feedstock m in region r, $m \in R_m$ and $r \in S_r$
$Tfix_{m,r,s}^{B}$ fixed transportation costs of feedstock m in region r with transportation mode s, $m \in R_m$, $r \in S_r$ and $s \in T_s$
$Tvar_{m,r,s}^{B}$ variable transportation costs of feedstock m in region r with transportation mode s, $m \in R_m$, $r \in S_r$ and $s \in T_s$
$Td_{m,r,i,s}^{B}$ transportation distance of feedstock m in region r to plant i with transportation mode s, $m \in R_m$, $r \in S_r$, $i \in Pa$ and $s \in T_s$

Plants

$PP_{m,i,k}$ product k price in plant i of feedstock m , $i \in I$, $m \in R_m$ and $k \in P$
$CPP_{m,i,g}$ co-product g price in plant i of feedstock m, $i \in I$, $m \in R_m$ and $g \in CP$
$eff_{m,i,k}^{Pa}$ yield of product k in plant i of feedstock m, $i \in Pa$, $m \in R_m$ and $k \in P$
$eff_{m,i,k}^{CPa}$ yield of co-product g in plant i of feedstock m, $i \in Pa$, $m \in R_m$ and $g \in CP$
$eff_{i,k}^{P}$ yield of product k in plant i, $i \in I$ and $k \in P$
c_i capacity plant i, $i \in I$
$CAP_{m,i,n}$ capital costs of plant i and size n using feedstock m, $i \in Pa$, $m \in R_m$ and $n \in PaSz$
$CAP_{i,n}$ capital costs of plant i and size n, $i \in I$ and $n \in N$
$OP_{m,i,n}^{fix}$ fixed operative costs of plant i and size n using feedstock m, $i \in Pa$, $m \in R_m$ and $n \in PaSz$
$OP_{i,n}^{fix}$ fixed operative costs of plant i and size n, $i \in I$ and $n \in N$
$OP_{m,i,n}^{var}$ variable operative costs of plant i and size n using feedstock m, $i \in Pa$, $m \in R_m$ and $n \in PaSz$
$OP_{i,n}^{var}$ variable operative costs of plant i and size n, $i \in I$ and $n \in N$
$T_{i,s}^{fix}$ fixed transportation costs from plant i with transportation mode s, $i \in I$ and $s \in T_s$
$T_{i,s}^{var}$ variable transportation costs from plant i with transportation mode s, $i \in I$ and $s \in T_s$
$Td_{i,j,s}$ transportation distance from plant i to plant j with transportation mode s, $i \in I$, $j \in I$, and $s \in T_s$

GHG abatement emissions

$e_{m,i}$ GHG emissions abatement in plant i using feedstock m, $i \in Pd$ and $m \in R_m$
e_s GHG emissions from transportation mode s, $s \in T_s$

Scalars

We present here constant values used in the optimization model.

Td_{CP} transportation distance co-product - *100 km*
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*
w_{EG} weight fraction of EG to produce PET – *0.3*
w_{TPA} weight fraction of TPA to produce PET – *0.7*
$\$_{carbon\ tax}$ carbon tax pricing – *25, 50, 100, 150 €/ton CO_2*

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

$x_{m,r,i}^{b}$ mass flow of feedstock m in region r to plant i, $m \in R_m$, $r \in S_r$ and $i \in Pa$
$x_{k,i,j}^{P}$ mass flow of product k from plant i to plant j, $k \in P$, $i \in I$ and $j \in I$
$x_{g,i}^{CP}$ mass flow of co-product g from plant i, $g \in CP$ and $i \in I$