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Comparative cradle-to-grave life cycle assessment of bio-based and petrochemical PET bottles

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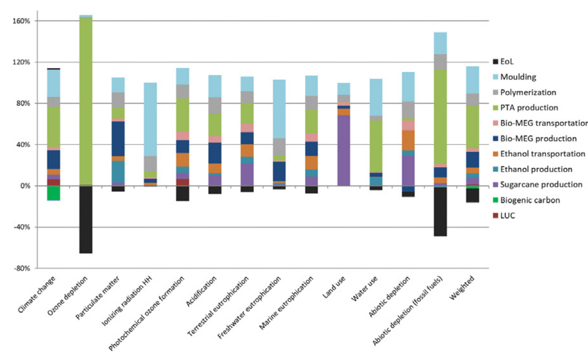
HIGHLIGHTS

- Life cycle assessment for bio-based PET bottles made with a cradle to grave scope.
- Beside sugar cane feedstock, European crops mix and wheat straw are studied.
- The impact of land-use change was included using a deterministic model.
- The end-of-life impacts were assessed using the EASETECH model.
- Bio-based PET bottles from wheat straw show similar performance with petrochemical PET bottles.

GRAPHICAL ABSTRACT



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ABSTRACT

This article presents a life cycle assessment of bio-based polyethylene terephthalate (PET) bottles with a cradle to grave scope and provides a comparison with petrochemical PET bottles for 13 environmental impact categories. Besides the baseline bio-based PET bottles, which are produced from Brazilian sugarcane reflecting status-quo, two alternative hypothetical bio-based product systems were considered: European wheat straw and European crops market mix composed of maize, wheat and sugar beet. The land-use change (LUC) impacts were assessed based on a deterministic model. The end-of-life impact was assessed using the EASETECH model. Baseline bio-based PET bottles performed overall worse than conventional petrochemical PET bottles, offering only better performance (about 10%) in abiotic depletion (fossil fuels). Comparable performance is observed for climate change (2% difference without the LUC, and 7% with LUC impacts). Using European crops for ethanol production (alternative 1) instead of Brazilian sugarcane resulted in a worse environmental performance, due to lower yields attained compared to Brazilian sugarcane. When wheat straw was considered as biomass feedstock for ethanol production (alternative 2), similar environmental performance with petrochemical PET bottles was seen.

1. Introduction

In the coming 20 years, the demand for plastics is expected to double globally (European Commission, 2018a). Plastics are the most widely used materials for packaging purposes due to their appealing

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characteristics (e.g. lightweight, transparent, flexible, good mechanical and barrier properties) (Mendes and Pedersen, 2021). An important part of packaging demand is generated by polyethylene terephthalate (PET) bottles (Euromonitor, 2019). In Europe, PET represents 7% of plastics consumption and is almost exclusively used for bottles (PlasticsEurope, 2018). There are sustainability issues associated with food and beverage packaging. The end of life of plastics, especially, raises environmental concern as well as fossil resource use (Geyer et al., 2017). Yet, there are strategies that could be applied to improve sustainability of packaging (Licciardello, 2017). For products characterized by a high packaging relative impact such as PET bottles, the most prominent strategies are weight and thickness reduction, and a shift to alternative materials such as bio-based plastics (Licciardello et al., 2015; Peelman et al., 2013).

Given the societal concern about climate change and fossil resource consumption, bio-based plastics have emerged as a possible solution produced from renewable resources (Coppola et al., 2021). Though they currently occupy about a 1% share of the plastics market, worldwide bioplastics production has been forecast to increase (Skoczinski et al., 2021). Bio-based PET represents approximately 8% of the global production capacity of bioplastics (Skoczinski et al., 2021). The use of bio-based PET for bottles accounts for more than 85% of the bio-based PET used globally with the rest finding use in technical (e.g. automotive, electronics) applications (Grand View Research, 2017).

PET is produced from monoethylene glycol (MEG), which accounts for approximately 30% by weight, and petrochemical purified terephthalic acid (PTA), which accounts for approximately 70% by weight. For the production of bio-based PET, petrochemical MEG is replaced by bio-MEG. The PTA part is still fossil-based. No commercial production of PTA from biomass currently exists. Several companies are working on the production of paraxylene from biomass which is the main precursor for PTA. However these technologies are not expected to become commercial in the near future (de Jong et al., 2020).

Bio-based PET is a drop-in product which is chemically identical to petrochemical PET and can therefore be recycled through the existing recycling systems. It can be reused and mechanically recycled together with petrochemical PET with no additional effort or negative impacts. For dedicated bio-based plastic products, on the other hand, there is no directly identical fossil-based counterpart. An example of this is polylactic acid (PLA) (Gironi and Piemonte, 2011). Although PLA can be mechanically recycled, this is currently not applied due to economic reasons which require a large volume of a certain plastic type to be available to be separately recycled.

Nevertheless, the name "bio-based" does not directly means that bio-based PET bottles are more environmentally friendly than petrochemical PET bottles (Chen et al., 2016). It is seen that there are sustainability challenges and trade-offs associated with the replacement of conventional plastics with bio-based in food packaging sector (Gerassimidou et al., 2021; Russell, 2014). As for other bio-based applications, it is, therefore, necessary to assess the potential environmental impact using an impartial methodology. One of the main tools used for evaluating the environmental performance of bio-based products is Life Cycle Assessment (LCA) (Giuntoli et al., 2019). LCA is a standardized method with two main international standards i.e. ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b). LCA allows accounting for the environmental burdens generated in the life cycle of a product from the extraction of raw materials to its end of life (ISO, 2006b). Accordingly, LCA allows making decisions on how to improve the sustainability of packaging from an informed and holistic foundation (Mendes and Pedersen, 2021).

This study aims to provide scientific evidence to support policymakers in their decisions about bio-based plastics (European Commission, 2018a; Giuntoli et al., 2019) by comparing, through LCA, the environmental performance of bio-based PET and petrochemical PET bottles. The Joint Research Centre of the European Commission is currently working on an LCA study on the potential environmental impacts of the use of alternative feedstocks (biomass, recycled plastics, CO_2) for plastic articles in comparison to using current feedstocks (oil and gas) where beverage bottles are one of the case studies (Nessi et al., 2020).

Despite the increased interest in bio-based plastics, only a few studies were conducted so far to assess the environmental performance of bio-based PET bottles. A recent review paper provides an overview of environmental impacts of bio-based plastics compared to fossil-based, where PET is one of the plastics being analysed (Walker and Rothman, 2020). The paper points out large variation in results mainly due to methodological differences between studies. Shen et al. (2011, 2012) carried out a comparative LCA of petrochemical PET, recycled PET, bio-based virgin PET and bio-based recycled PET (Shen et al., 2012, 2011). Ethanol used in the production of bio-based PET in the studies was based on maize-derived from the US and sugarcane-derived from Brazil. The assessment was limited to greenhouse gas (GHG) emissions and non-renewable energy use (NREU) impact categories and data was attained from Chen and Patel (2012) (Chen and Patel, 2012). Bio-based PET was found to allow significant reduction in GHG emissions and NREU (about 20%) compared to petrochemical system, and even larger savings were seen considering recycled system (Shen et al., 2011). It was seen that the comparison was sensitive to the allocation method applied to open-loop recycling (Shen et al., 2012). The impacts estimated for bio-based PET were considered to be low and this was explained to be due to authors using stoichiometric yields to ethanol requirement for ethylene, theoretical heat of formation for energy requirement for dehydration, and not considering the production of bio-MEG taking place in India (related transport demands and energy production intensities) (Tsiropoulos et al., 2015). Tabone et al. (2010) carried out assessment for bio-based PET with a cradle to gate scope for TRACI impact categories and found to have unfavourable performance compared to petrochemical PET (Tabone et al., 2010). The bio-based PET inventory was modelled using background data from Ecoinvent database. This paper was used as reference and adjusted in the assessment carried out by Hottle et al. (2017) which also included end of life stage (Hottle et al., 2017). Akanuma et al. (2014) provided a preliminary comparison of three pathways for bio-PTA production for 100% bio PET syntheses (Akanuma et al., 2014). The assessment had a cradle to gate scope and IMPACT 2002+ method was used for impact assessment. The production was modelled using US life cycle inventory data where bio-MEG production from maize was considered and data were obtained from Ecoinvent. These earlier studies are considered to provide rough estimate of environmental impact of bio-based PET bottles and they do not provide breakdown of the impact to the process stages involved.

Tsiropoulos et al. (2015) carried out a cradle to gate assessment of bio-based PET from sugarcane ethanol (from Brazil or India) using IMPACT 2002+ method (Tsiropoulos et al., 2015). They found similar performance to petrochemical PET bottles in term of GHG emissions. Industry-based data (from technology licensors or producers) was acquired for the different stages of bio-MEG production which resulted in highly representative data to be utilized in the assessment. Therefore, this paper was selected as reference for bio-MEG production inventory in this paper. In a recently published study by Chen et al. (2016) various bottles made from 100% bio-PET, bio-based PET and fossil-based PET were compared using an attributional LCA with a cradle-to-gate scope (Chen et al., 2016). They used inventory data reflecting U.S. context where corn, switchgrass and wheat straw were considered as raw materials for bio-MEG. For the impact assessment, they used TRACI v2.1 developed specifically for U.S. conditions analysing eight impact categories. Conversely, in this article, we aim to reflect on the context of European industries and an assessment considering the whole life cycle. Accordingly, the European Product Environmental Footprint (PEF) method (Manfredi et al., 2012) was followed for impact assessment with 13 impact categories. For reliable comparison of results, it was recommended in a recent review paper to follow this PEF method (Walker and Rothman, 2020). In the paper, end-of-life impacts are included representing current European practice and additional cases for European crops and wheat straw as potential feedstocks were considered.

Valorization of agricultural residues is important for circular bio-based economy. Their utilization increases resource efficiency and allows reducing over-exploitation of natural resources (Ingrao et al., 2021). Use of agricultural residues for bio-based PET production was also considered in previous studies (wheat straw by (Chen et al., 2016) and corn stover by (Benavides et al., 2018)). Wheat straw is one of the agricultural residues identified to have high potential for biofuel and biochemical applications (Sarkar et al., 2012). One of the key obstacles is the high cost for straw collection and transportation, as well as quality control of the straw (Sun et al., 2020). Additionally, agricultural residues should not be considered burden-free and environmental consequences of diversion of these sources (e.g. nutrient losses in the soil) need to be accounted for in assessing the sustainability of a given use (Tonini et al., 2016).

2. Materials and methods

The LCA was carried out based on the ISO 14040:2006 and ISO 14044:2006 (ISO, 2006a, 2006b) standards. Moreover, to a large extent, the recommendations of the draft Product Environmental Footprint Category Rules (PEFCR) guidance, version 6.3 (European Commission, 2018b) were followed.

2.1. Goal and scope definition

2.1.1. Goal and functional unit

The goal of this case study was to assess the environmental profiles of selected pathways for bio-based PET beverage bottles and compare them with (conventional) petrochemical PET bottles.

The function of a beverage bottle is to hold a certain amount of beverage. Packaging of water is the most important application for PET bottles representing over 40% of all soft drink volume. The share of water bottles is forecasted to increase further (Euromonitor, 2019). In 2015, ca. 41% of all PET bottles used for packaging water had a volume of 0.5 L and less, ca. 33% had between 1 and 3 L volume. The remaining quarter had larger than 3 L volume (Nestlé Waters, 2015). Accordingly, as the most representative product sold in the market, the functional unit of this case was defined as *packaging water in one hundred 0.5 L bottles providing a shelf life of at least 9 months*.

The average weight of a 0.5 L water bottle weighs about 10 g (PETRA, 2017). As a result, this functional unit equals 1 kg of PET bottles. It is important to note that this is nearly half of what a typical 0.5 L bottle weighed in 2000 (18.9 g) and there are ongoing efforts to further reduce the bottle's weight (Nestlé Waters, 2015). The mass associated with the functional unit is identical for both the bio-based and the petrochemical PET bottles because they are chemically identical.

2.1.2. Product systems

A so-called "baseline" bio-based pathway was defined to reflect the status-quo commercial production of the bio-based PET product. Next to this baseline, alternative scenarios were also explored to evaluate the impact of using alternative biomass feedstocks.

The baseline pathway is the production of bio-based PET using Brazilian sugarcane. This was selected because currently, only one company produces bio-MEG on a large industrial scale for incorporation into PET, and its production takes place in India at India Glycols (de Jong et al., 2020). This company produces bio-MEG from ethanol. Although ethanol can be produced from various biomass feedstocks, sugarcane is currently the only feedstock used in the production of bio-MEG. Brazilian sugarcane is used as feedstock in this study since Brazil is the world's largest sugarcane and sugarcane-based ethanol producer. It should be noted that India Glycols also use ethanol produced from Indian sugarcane molasses in their bio-MEG plant, but this ethanol is not considered in this study.

Furthermore, two alternative fictive bio-based PET pathways were considered. The first one considers using European ethanol instead of Brazilian ethanol. In Europe, approximately 90% of the fuel ethanol is made from maize, wheat and sugar beet (ePURE, 2017). The combined market mix was considered where 36% of ethanol is produced from maize, 37% from wheat and 27% from sugar beet.

The second alternative feedstock considered for ethanol production was European wheat straw to include the possibility of using lignocellulosic biomass instead of crops as a source. There is ongoing fast development for commercial-scale 2nd generation ethanol from straw (Bakker et al., 2013; ePURE, 2017; Obydenkova et al., 2017). However, sugar production from lignocellulosic biomass needs to be further developed to become cost-competitive with 1st generation ethanol from sugar and starch crops. This is important in achieving a sustainable transition in the chemical industry from fossil to biomass feedstocks.

These three bio-based pathways are compared with the reference system of petrochemical PET bottles with a European industry context.

2.1.3. Scope

The geographical scope is Europe for the purchase, use and disposal of the PET bottle. However, the study considers all processes occurring outside Europe prior to purchase (e.g. feedstock cultivation and harvesting and conversion processes). For the baseline, the cultivation of sugarcane and its conversion to ethanol takes place in Brazil. For the alternative feedstock systems, wheat, maize, sugar beet and wheat straw are sourced and converted to ethanol in Europe. The conversion of ethanol to bio-MEG takes place in India. The PTA and bottle grade PET production and stretch blow moulding processes occur in Europe.

The temporal scope is current production with relevant developments foreseen for the short-time future (5–10 years). The production of ethanol from lignocellulosic feedstock has recently become commercialized and more development is expected in the near future (Obydenkova et al., 2017). Currently, only sugarcane-based ethanol is used for bio-MEG production. The conversion of ethanol produced from the two alternative biomass feedstocks to bio-MEG represents fictive scenarios although it considers the same technology since the ethanol used is chemically identical.

A cradle-to-grave system boundary was used including the life cycle stages of feedstock production, manufacturing and end of life (EoL). The consumer use phase is excluded from the analysis which is the same for all product systems and has a negligible impact.

2.1.4. Impact categories and assessment methods

Given the aim to support European Union (EU) policy-making, the selection of the impact categories was based on the recommendations of PEFCR guidance version 6.3 (European Commission, 2018b) with the exclusion of toxicity impact categories (human toxicity, cancer; human toxicity, non-cancer and ecotoxicity, freshwater) whose methods are still under development and review (Zampori et al., 2016). PEFCR guidance excludes the toxicity impact categories in the procedure of identifying the most relevant impact categories and total environmental impact is determined with weighting using these 13 impact categories. Table A.1 provides the 13 impact categories considered and their assessment methods. Normalization and weighting factors were used in identifying the most relevant unit processes and impact categories (that contribute the most to the total normalized and weighted environmental impacts) for each product system.

Eight impact categories were found suitable to be used for the comparison with petrochemical PET bottles. Some categories were excluded in the comparison due to the significant differences in the life cycle inventories of the publicly available datasets for petrochemical PET[1] (e.g. more than 50% of impact difference in the impacts calculated).

[1] The datasets published by PlasticsEurope's (used in our modelling) and GaBi 2017 database for PET were compared. The geographic scopes of the two datasets were not the same (average Europe for PlasticsEurope vs. Germany for Gabi). However, the important differences observed cannot be linked mainly to the geographical scope but more to the lack of harmonization in the data categorisation and inventory modelling.

Table 1
PET bottle pathways considered in this study.

Product system	Processes	Data sources	Comments
Baseline	Sugarcane cultivation and harvest	(Tsiropoulos et al., 2014)	Represents south-central Brazil, reference year 2008, based on CTC data found in the paper of (Seabra et al., 2011).
	Bioethanol production from sugarcane	(Tsiropoulos et al., 2014)	Represents south-central Brazil, reference year 2008, based on CTC data found in the paper of (Seabra et al., 2011).
	Bio-MEG production	(Tsiropoulos et al., 2015)	Represents production in India in 2011 based on proprietary data from industrial producer
	PTA production (fossil)	Industry data 2.0 and (PlasticsEurope, 2017).	Industry data 2.0 process with climate impact modified based on the most recent PlasticsEurope report representative of European average, reference year of 2015.
	Esterification and Polymerisation	Ecoinvent 3.3 and (PlasticsEurope, 2017).	Ecoinvent 3.3 process with climate impact modified based on the most recent PlasticsEurope report representative of European average, reference year of 2015.
	Stretch blow moulding	Ecoinvent 3.3 and (Kuczenski and Geyer, 2011)	Ecoinvent 3.3 process with electricity consumption modified to 6.1 MJ/kg.
Alternative 1	Wheat, maize and sugar beet cultivation and harvest	AgriFootprint, 2017	Represents national cultivation practices for the European countries and crops, weighted average European inventory calculated based on Eurostat (EUROSTAT, 2017a).
	Wheat and maize drying	(Edwards et al., 2017)	The average % of water removed based on CAPRI database (CAPRI, 2016)
	Bioethanol production from wheat	(Buchspies and Kaltschmitt, 2017) and (BioGrace-I, 2015)	Represents industrial production in Europe.
	Bioethanol production from maize	(Edwards et al., 2017)	Represents industrial production in Europe.
	Bioethanol production from sugar beet	(Buchspies and Kaltschmitt, 2017)	Represents industrial production in Europe.
Alternative 2	Wheat straw	(Tonini et al., 2016)	The amount of mineral fertilizers based on nutrient content and method provided in this source
	Straw baling	(Giuntoli et al., 2017)	Represents European production
	Bioethanol production from wheat straw	(Edwards et al., 2017)	Represents European production data based on (Johnson, 2016)
Petrochemical	Petrochemical MEG production	Ecoinvent 3.3 and (PlasticsEurope, 2017).	Modified Ecoinvent 3.3. process with climate impact calculated based on the most recent PlasticsEurope report representative of European average, reference year of 2015.

Moreover, some impact categories were not found applicable because PlasticsEurope's ecoprofiles do not distinguish between emissions to fresh water and to seawater making it impossible to determine the freshwater eutrophication.

2.2. Life cycle inventory analysis

2.2.1. Method used for handling multifunctional systems

Following the ISO 14044:2006 standard, for multi-output processes, allocation is avoided whenever possible by system expansion or subdivision (ISO, 2006b). As described in the International Reference Life Cycle Data System (ILCD) handbook system expansion can mean to add another, not provided function to make to system comparable (i.e. system expansion in the stricter sense) or to subtract the additional functions of the system, i.e. by substituting them by the ones that are replaced (i.e. substitution by system expansion) (European Commission et al., 2010). The substitution method was applied in this study. Substitution means to subtract the inventory of another system from the analysed system. In the following sections, the details on co-products and substituted processes can be found for each specific product system along with inventory data.

2.2.2. Method used for accounting of biogenic carbon

The climate change from cradle-to-gate is calculated as the sum of fossil GHG emissions and biogenic non-CO_2 GHG emissions minus the biogenic carbon embedded in the product. Based on the molecular structure of PET and the biogenic carbon content coming from MEG, the biogenic carbon embedded in the bio-based PET bottle is calculated as 0.45 kg CO_2/kg for bio-based PET. In the EoL stage, the carbon is (partially) emitted again based on the EoL option and a net balance is calculated for the cradle-to-grave system.

2.2.3. Inventory data

The life cycle inventory of bio-based PET bottles includes data for the key unit processes of biomass cultivation and harvesting, ethanol production, bio-MEG production, PTA production, PET production (esterification and polymerisation) and stretch blow moulding with transportation processes in between. These are explained in the sections below for each product system investigated and an overview of the foreground data sources is provided in Table 1. For background data, e.g. grid electricity and heat, other utilities and production of chemicals and materials, Ecoinvent 3.3 is used. The modelling of land-use change and end-of-life are described separately in Sections 2.3 and 2.4 respectively.

2.2.4. Bio-based PET bottles from Brazilian sugarcane (baseline)

Fig. 1 illustrates the flow diagram for bio-based PET bottles (baseline) showing the unit processes involved, counterfactual processes and the end of life options.

The first unit process in this product system is sugarcane cultivation and harvest in Brazil. Once harvested, sugarcane is transported to ethanol plants. For this unit process, data was retrieved from (Tsiropoulos et al., 2014). As shown in Fig. 1, a unit process that combines sugarcane processing, ethanol production and the combined heat and power (CHP) was modelled. The inventory data for sugarcane cultivation and harvest and ethanol production were retrieved from (Tsiropoulos et al., 2014). The data is representative of the production in south-central Brazil, which is responsible for about 90% of the sugarcane production in Brazil. The data is from the database of the sugarcane technology center (CTC) as reported in (Seabra et al., 2011).

This is the most recent, comprehensive and reliable data publicly available and used as a reference in many recent publications concerning GHG emission calculations and LCA including (Tsiropoulos et al., 2014). However, this industry-based data is for the 2008/2009 season where 65% of the areas had burned cane harvesting. The São Paulo State Law (n. 11,241/2002) established that the practice of burning must be completely eliminated by 2021 in mechanized areas, and by 2031 in non-mechanized areas with slopes greater than 12% (Carvalho et al., 2017). In the Center-South region, more than 90% of the area is already mechanically harvested (mostly unburned cane) (Conab, 2020). In order to better represent the current conditions where trash burning is phased out, the inventory data is modified to remove trash burning-

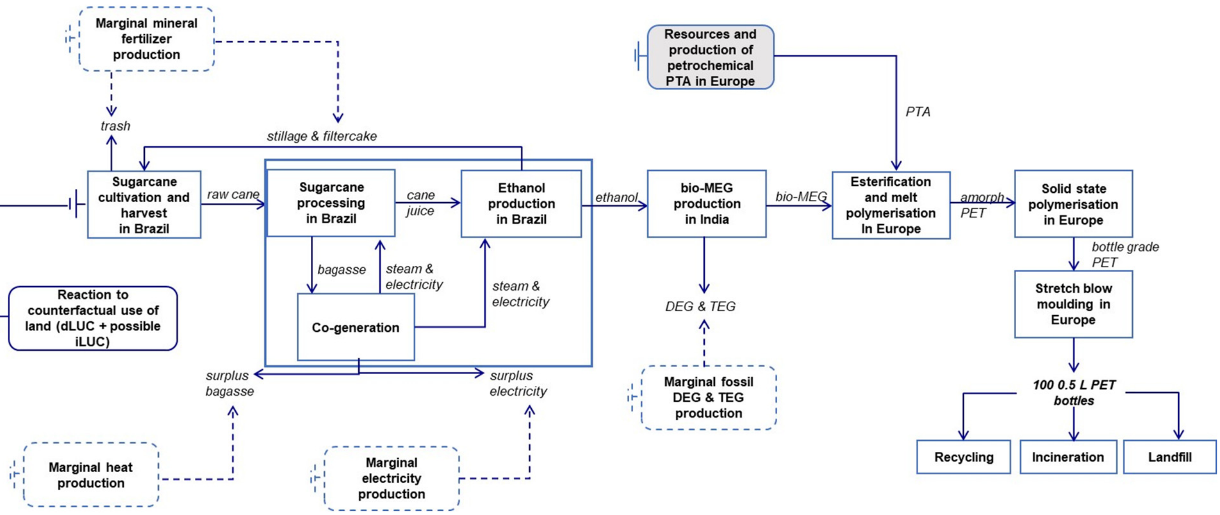

Fig. 1. Process flow diagram for bio-based PET bottles (baseline). Dashed boxes represent the expansion of the boundaries to include counterfactual unit processes such as marginal replacements of co-products and the impact of land use change.

related emissions from air emissions. Further description is provided in the supplementary information.

In ethanol plants, the juice is extracted from sugarcane and processed through fermentation. After fermentation, the broth goes through distillation and rectification to purify ethanol. From the juice extraction process, bagasse is obtained as a residue. Bagasse is burned in a CHP plant to supply the heat and electricity demand of the ethanol plant with the electricity surplus (0.16 kWh/kg ethanol) sold to the grid (Edwards et al., 2017; Tsiropoulos et al., 2014). In the market, this surplus of electricity replaces marginal electricity production and supply to the grid, which, for Brazil is considered to be electricity from natural gas as described by (Seabra et al., 2011). The process produces also an excess of bagasse (8.7 kg/t sugarcane) that is sold to the market and used by industries as fuel (Seabra et al., 2011). The heat produced from bagasse is considered to replace heat production from light fuel oil in Brazil (0.9 MJ/kg ethanol) as described in (Tsiropoulos et al., 2014). Other residues are filter cake and stillage which are returned to sugarcane fields and applied as fertilizers (Tsiropoulos et al., 2014). Therefore, they are consumed within the system boundaries.

The bioethanol produced in Brazil is then transported to India where the conversion to bio-MEG occurs. In India, bio-MEG is produced through four processes in series i.e. ethanol dehydration to ethylene, ethylene oxidation, hydration of ethylene oxide to ethylene glycols and distillation. For the bio-MEG production process, data were retrieved from (Tsiropoulos et al., 2015). During the distillation process, diethylene glycol (DEG) and triethylene glycol (TEG) are produced as minor by-products and are assumed to be substituting fossil-based diethylene glycol and triethylene glycol in the market. Data for these were retrieved from Ecoinvent 3.3. Bio-MEG produced in India is then sent to Europe. The distances and modes for transporting ethanol to bio-MEG plant and transporting of bio-MEG from plant to Europe were retrieved based on (Tsiropoulos et al., 2015).

The other main ingredient for bio-based PET i.e. fossil-based PTA is produced in Europe. For PTA, the dataset of PlasticsEurope's PTA eco-profile was used (PlasticsEuope, 2014). PET is then produced by esterification of bio-MEG with fossil-based PTA. Amorphous PET is then obtained via melt polymerisation and upgraded into bottle-grade PET via solid-state polymerisation. The impact of esterification and polymerisation was retrieved using the Ecoinvent 3.3 database. Both for PTA production and polymerisation, the climate change impact is updated with the breakdown given in the latest PlasticsEurope PET eco-profile (PlasticsEurope, 2017). Further description is provided in the supplementary information.

PET bottles are produced through stretch blow moulding. The Ecoinvent 3.3 dataset was used for this process with key activity level data of electricity consumption modified to a more conservative value (6.1 MJ/kg) based on a literature review (Kuczenski and Geyer, 2011).

2.2.5. Bio-based PET bottles from European crops (Alternative 1)

This product system (Fig. 2) uses ethanol mix produced from European crops instead of ethanol from Brazilian sugarcane for the production of bio-MEG. The main crops used to produce ethanol in Europe are maize, wheat and sugar beet (forming together approximately 90% of ethanol production (ePURE, 2017)). The market mix of ethanol from these three crops is considered as feedstock as described in Section 2.1.2.

In this fictive bio-based PET pathway, the unit processes following ethanol production are considered to be the same as the baseline bio-based PET product system. Therefore, below only the unit processes of biomass cultivation and harvest and ethanol production are described.

For determining the weighted average European inventory for each crop, Eurostat statistics were collected and averaged over 5 years (2013 to 2017) (EUROSTAT, 2017a). Based on this, average European production was made for each crop with representativeness over 80% of the total European production. Data on the contribution of the EU countries in the modelled average European maize, wheat and sugar beet is provided in supplementary information.

Agrifootprint database was used to retrieve the inventory data for the national cultivation practices for the relevant countries and crops. Then the shares were used to calculate the weighted average European inventory for each crop.

Wheat and maize are dried before transport. The average percentage of water removed based on CAPRI database (CAPRI, 2016) is 0.2% for wheat and 6.1% for maize (Edwards et al., 2017). The crops are transported to ethanol plant by truck. The transportation distances were assumed as 30 km for sugar beet and 100 km for wheat and maize (Edwards et al., 2017). For bio-ethanol production from maize in Europe, the inventory data was retrieved from (Edwards et al., 2017). For wheat, data from Biograce tool (BioGrace-I, 2015) was used in combination with (Buchspies and Kaltschmitt, 2017) for the chemical inputs. Wheat and maize are milled in a dry milling process. Then, ethanol is produced via hydrolysis and fermentation. Subsequently, the ethanol produced via fermentation is separated from water and impurities by distillation and dehydration. From distillation, stillage is obtained and once dried can be sold as dried distiller grains with solubles (DDGS) for animal feed. DDGS from wheat and maize displace a mix of marginal

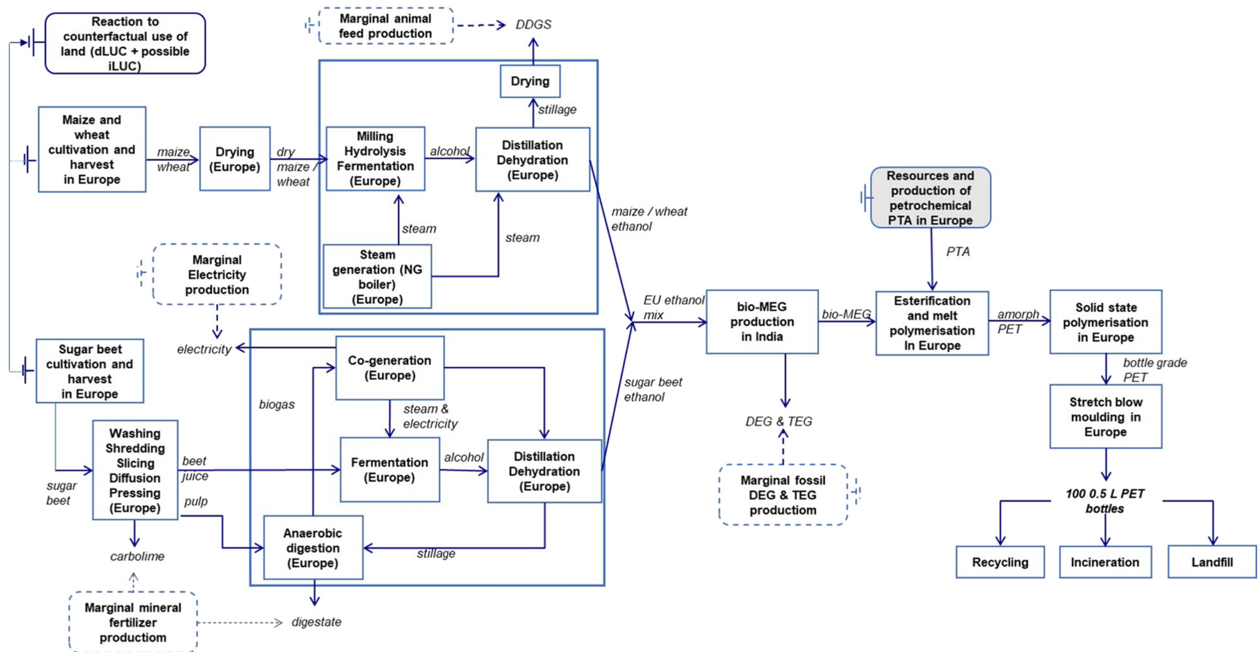

Fig. 2. Process flow diagram for bio-based PET bottles derived from European crops (alternative 1). Dashed boxes represent the expansion of the boundaries to include counterfactual unit processes such as marginal replacements of co-products and the impact of land-use change.

feed ingredients with the same standardized feed unit (further information provided in supplementary information). Based on near-future demand trends from (FAO, 2014; FAPRI U.S., 2012), soybean meal was selected as marginal protein, maize as marginal carbohydrate and palm oil as marginal oil as explained in (Tonini et al., 2016).

For bioethanol production from sugar beet in Europe, the data reported in (Buchspies and Kaltschmitt, 2017) was used. Once harvested, sugar beet is washed, sliced and pressed. As a result, beet juice is produced along with beet pulp and carbonation lime. Ethanol is produced from beet juice via fermentation followed by distillation and dehydration. The distillation process delivers stillage as a by-product. Beet pulp along with stillage are used to produce biogas which is used for the internal supply of heat and electricity plus an electricity surplus sold to the grid (replacing EU medium voltage electricity). Digestate from anaerobic digestion and carbonation lime are used as fertilizer. Accordingly, they displace a mix of marginal N, P and K fertilizers based on their nutrient contents attained from (Buchspies and Kaltschmitt, 2017). Based on the trends in the demand reported in (Tonini et al., 2016), urea, diammonium phosphate (DAP), and potassium chloride were selected as the marginal N, P, and K fertilizers respectively. Detailed values for the displacements used in this study are provided in the supplementary information.

European ethanol market mix is accordingly made consisting of 36% ethanol from maize, 37% from wheat and 27% from sugar beet as described in Section 2.1.2. This representative European ethanol is then transported to India for conversion into bio-MEG. From this process onward, the processes are the same as the baseline bio-based PET product system.

2.2.6. Bio-based PET bottles from European wheat straw (Alternative 2)

The second (fictive) alternative bio-based PET product system (shown in Fig. 3) uses ethanol from European wheat straw. Also, in this fictive bio-based PET pathway, the unit processes following ethanol production are considered to be the same as the baseline bio-based PET product system. Only the unit processes of wheat straw supply and ethanol production are described below.

Wheat straw is a residue left on the field after wheat grains harvesting. In the last decade, it has received attention as an important feedstock for second-generation ethanol. However, removing the wheat

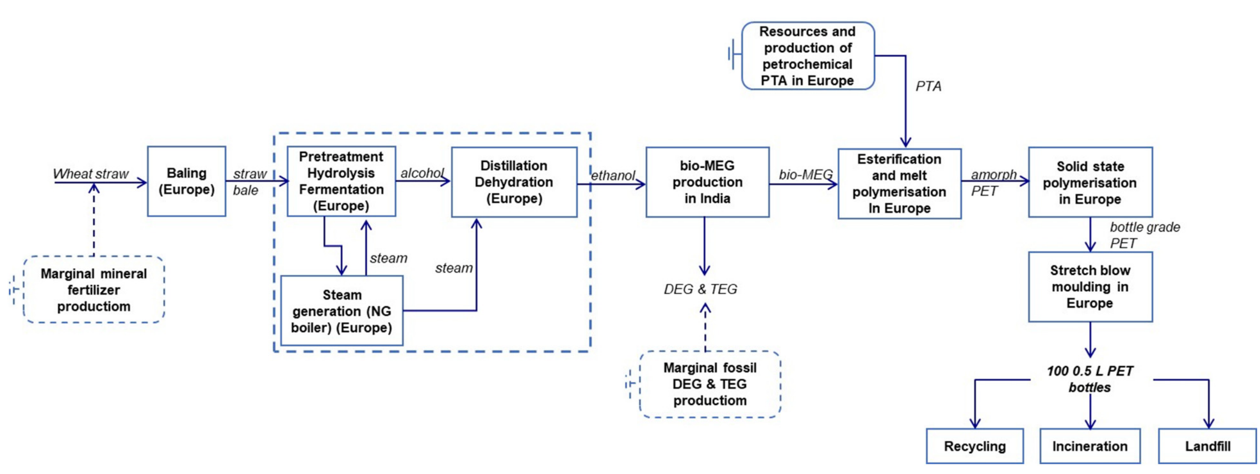

Fig. 3. Process flow diagram for bio-based PET bottles derived from European wheat straw (alternative 2). Dashed boxes represent the expansion of the boundaries to include counterfactual unit processes such as marginal replacements of co-products and the impact of land-use change.

straw from the field can have consequences on the nutrient management of the soil which needs to be accounted for. Removal of wheat straw from land would require additional N, P and K mineral fertilizers to be applied in accordance with the contents of the wheat straw to avoid soil depletion. The nutrient contents of wheat straw were retrieved from (Tonini et al., 2016). As explained above, urea, DAP, and potassium chloride were selected as the marginal N, P, and K fertilizers respectively. Detailed values for the displacements used in this study are provided in the supplementary information.

Data for straw baling and transport was retrieved from (Giuntoli et al., 2017) and data for the subsequent ethanol production was retrieved from (Edwards et al., 2017). Before fermentation, wheat straw goes through pre-treatment and hydrolysis to produce sugars. The solid by-products from this process are used to produce heat, which is consumed internally. Ethanol is produced from the sugars via fermentation followed by distillation and dehydration.

2.2.7. Petrochemical PET bottles

For the pathway representing petrochemical PET bottles, the most recent eco-profile released by PlasticsEurope for bottle-grade PET was considered as the main reference (PlasticsEurope, 2017). This eco-profile represents the current average industrial production of PET in Europe with coverage of about 85% of the installed production capacity. The individual life cycle inventory (LCI) datasets were collected from participating companies for the reference year 2015 and due to confidentiality vertical averaging was applied. It is indicated that where necessary processes have been allocated by physical properties, such as mass, energy, or enthalpy. Because data is exclusively presented as aggregated, it was not possible to identify the most important activity level data for the potential environmental impacts.

To be consistent with the modelling for the bio-based PET product systems, it is important to have the breakdown for all unit processes, therefore we opted to model our own petrochemical PET product system. The petrochemical PET bottle product system involves the unit processes, petrochemical MEG and petrochemical PTA production, polymerisation and stretch blow moulding. The processes of PTA production, polymerisation and stretch blow moulding are the same as the bio-based product system as described in Section 2.2.4.

The CML impact assessment method is used in PlasticsEurope PET ecoprofile where only for the climate impact category same assessment model (i.e. (IPCC, 2013)) as in this study is used. Thus, for the remaining impact categories, it was required to use data from the databases Industry data 2.0 from PlasticsEurope (PlasticsEurope, 2011) and Ecoinvent 3.3. For PTA, the dataset of Industry data 2.0 was used. For petrochemical MEG, the dataset of Ecoinvent 3.3 was used. The impact of polymerisation was retrieved using the Ecoinvent 3.3 database. For all, the climate change impact is updated with the breakdown given in the latest PlasticsEurope PET eco-profile (PlasticsEurope, 2017). These data were compiled to form the petrochemical PET data in this study using reaction stoichiometry which states 0.32 kg MEG and 0.86 kg PTA per kg PET. Further description and breakdown are provided in the supplementary information.

2.3. Modelling of land-use changes

In this study, the impact of displacing land as additional arable land demanded i.e., the so-called land-use changes (LUC), for sugarcane cultivation in Brazil, and wheat, maize and sugar beet cultivation in EU were taken into account. The PEFCR method does not cover indirect land-use change (ILUC). Instead, ILUC is modelled based on the approach described in (European Commission, 2019) updating the deterministic approach presented in (Tonini et al., 2016). It is based on an analysis of the global deforestation that occurred between 2000 and 2010, and considers two key reactions to an increased demand for arable land, namely arable land expansion (85% of the response) and agricultural intensification (15% of the response; here translated as an additional fertilizer demand only). These two shares are based on (Marelli et al., 2011). Further description of the land-use change model is described in Moretti et al. where it was applied to assess LUC impacts of PLA cups (Moretti et al., 2021).

The LUC implications of PET bottle production were derived using the dry matter (DM) yield of the crops included in this study: 22.7 megagram (ton) of dry matter per hectare (Mg DM ha^{-1}) used for Brazilian sugarcane and average 11 Mg DM ha^{-1} for EU crops (considering the share of wheat, maize and sugar beet in the ethanol mix, and the EU country mix where these crops stem from).

2.4. Modelling of end of life

Based on the EU statistics of waste treatments of waste plastics (European Commission, 2018a), the end of life of PET bottles is modelled as 60% recycling, 20% incineration and 20% landfilling. Since bio-based PET bottles are chemically identical, the EoL impacts are the same as for the petrochemical bottles. The end of life processes of mechanical recycling, incineration and landfilling were modelled using the processes incorporated in the EASETECH model (Clavreul et al., 2014). Compared to other LCA software, EASETECH offers the possibility to account for the exact composition of the material flows (Clavreul et al., 2014). The key parameters that were modified compared to EASETECH standard processes are described below.

For PET bottles, the materials flows were determined based on the chemical composition of PET bottles plus the organic contamination that accompanies the bottles during the waste management. In particular, the composition of the waste flow (contaminated PET waste) was based on (Götze et al., 2016), who measured the chemical composition of various municipal solid wastes in Denmark. This flow has a moisture content of 3.3%, volatile solids make up 99% of solids and the carbon content is 64% of the total solids (Götze et al., 2016).

Mechanical plastic recycling process includes the energy and material requirements for the transportation to the facility, sorting, cleaning and recycling processes. The recycled PET is assumed to substitute virgin PET production. The efficiency (including sorting) was taken to be 76% (Plastics Recyclers Europe, 2017) and the remaining rejects are treated with incineration. The life cycle inventory data for mechanical recycling were retrieved from (Rigamonti et al., 2014) and petrochemical bottle grade PET data from PlasticsEurope (PlasticsEurope, 2017) was used to calculate the credit from the substitution of virgin PET.

The incineration process includes the direct emissions from waste incineration as well as indirect emissions from the production of the input materials, combustion of fossil fuels as well as treatment of bottom ash and fly ash. For incineration, the average heat efficiency of 22% and electrical efficiency of 9% were used based on average EU municipal solid waste incineration (MSWI) data from 314 waste incineration plants of which 60% with energy recovery units (EUROSTAT, 2017b; Reimann, 2012). The average efficiencies of the MSWI plants with energy recovery are 15% electrical efficiency and 35% heat efficiency (EUROSTAT, 2017b; Reimann, 2012). The marginal EU electricity was based on (Itten et al., 2014) updated with 2017 data. The marginal EU heat was assumed produced from natural gas using Ecoinvent 3.3 data.

For landfilling, EASETECH standard process was used. This process includes the construction and operation of the landfill site, direct emissions of landfill gas, landfill gas collection, flaring and recovery system, treatment of collected leachate and direct emissions from uncollected leachate. 29% of the collected landfill gas was taken to be used for electricity generation (OpenLCA Nexus, 2015) with electrical efficiency of 37% (Christensen, 2010).

3. Results

3.1. Bio-based PET bottles from Brazilian sugarcane (baseline)

The breakdown of the cradle-to-grave impact of bio-based PET bottles (baseline) per functional unit of 1 kg is presented in Fig. 4

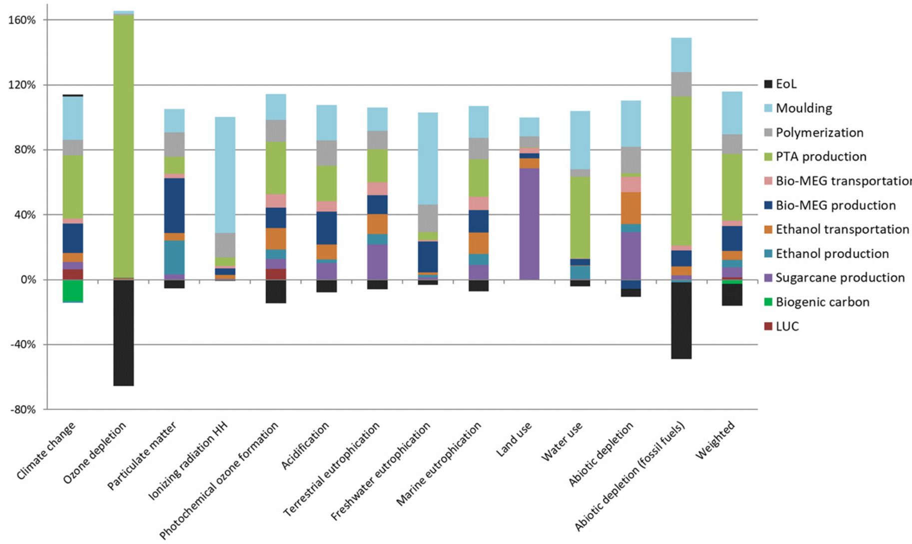

Fig. 4. Breakdown of the cradle-to-grave impact of bio-based PET bottles from Brazilian sugarcane (Baseline) per functional unit.

(Table with background values is provided in the supplementary information).

The most relevant impact categories (i.e. the ones contributing the most to the total normalized and weighted environmental impacts) are particulate matter, climate change and abiotic depletion (fossil fuels) with contributions in the range of 16–19% (see supplementary information Table S18). In Fig. 4, the impacts are broken down into the main unit processes described in Section 2.2.4. The most relevant life cycle stage is manufacturing, followed by biomass cultivation and harvest. The most relevant unit processes in manufacturing stage are PTA production followed by moulding which have 41% and 26% contribution respectively to overall weighted environmental impacts. It is seen that for climate change and abiotic depletion (fossil fuels) impacts, PTA production is dominating. This is due to the use of fossil inputs (predominantly crude oil and natural gas) as feedstock and for process energy demands. Looking at the dominance analysis of most recent PTA eco-profile of PlasticsEurope (PlasticsEurope, 2016), p-xylene production and the related upstream processes is responsible for the majority of impacts (>60%) concerning these impact categories. At EoL stage, savings are achieved in almost all impact categories with major savings observed for the ozone depletion and abiotic depletion (fossil fuels). This is owing to the substitution of virgin plastic impacts achieved with recycling and heat and electricity substitution with incineration. Since PTA production, polymerisation, moulding and EoL processes are identical in both bio-based and petrochemical product systems, the contributors for the unit processes for bio-MEG production are analysed further below.

Looking at sugarcane cultivation and harvest, it contributes 6% to the weighted results. This process has an important contribution on the land use (69%) and also on abiotic depletion (29%) and terrestrial eutrophication (22%) categories related to fertilizer application. Bioethanol production does not have a significant contribution (5% to the weighted results). This is mainly due to the use of the by-product bagasse for internal energy supply and the credits gained by the surplus electricity and bagasse. Significant contribution of bio-MEG production is seen especially for climate change, particulate matter and acidification. For these, most of the impact is caused by the production of the energy used in the process i.e. mainly coal-based electricity and steam production in India.

Concerning the land use change impacts, they contribute only to 2% of the total cradle to grave impact on weighted bases. LUC show about 6–7% contribution to climate change and photochemical ozone formation. The climate change impact of LUC is due to carbon dioxide resulting from land clearing while the photochemical ozone formation impact is mainly caused by carbon monoxide also released during land clearing. LUC processes are dependent on the amount of land needed. Therefore, considering a higher yield than 22.7 Mg DM ha^{-1} used in this study would result in lower impacts.

3.2. Bio-based PET bottles from European crops (Alternative 1)

The breakdown of the cradle-to-grave environmental impact of bio-based PET bottles from European crops (alternative 1) per functional unit of 1 kg is shown in Fig. 5 (Table with background values is provided in the supplementary information).

The most relevant impact categories are climate change and abiotic depletion (fossil fuels), followed by particulate matter (see supplementary information Table S18). In Fig. 5, the impacts are broken down into the main unit processes described in Section 2.2.5. This alternative bio-based PET product system differs from the baseline in the following unit processes: EU crops production, ethanol production, ethanol transportation and LUCs. The production of the EU crops contributes to 20% of the overall weighted impact with high contributions seen for the impact categories land use, marine eutrophication and terrestrial eutrophication. Nitrate emissions to water and nitrogen oxides emissions from fertilizer application are the main sources of impact on marine eutrophication. The impact on terrestrial eutrophication is mainly due to ammonia and nitrogen oxides emissions caused by the fertilizer application.

On weighted bases, ethanol production from EU biomass crops represents a credit of 4% on the total cradle-to-grave impact mainly resulting from the by-product DDGS from wheat and maize processing displacing a mix of marginal feed ingredients (soybean meal, maize and palm oil). In particular, the avoidance of animal feed production allows major savings in the land use and abiotic depletion (due to avoided application of fertilizers and pesticides) categories.

LUC contributes to 14% of both the impact on climate change and photochemical ozone formation (two impacts dominated by land expansion) and to 4% of the total cradle-to-grave impact on weighted bases. This is due to the carbon dioxide and carbon monoxide released from land clearing as was in the baseline (Brazilian sugarcane). However, higher LUC impacts are observed in this product system. The reason why European crops generate higher LUC impacts than Brazilian sugarcane can be found in the amount of land needed i.e. the greater

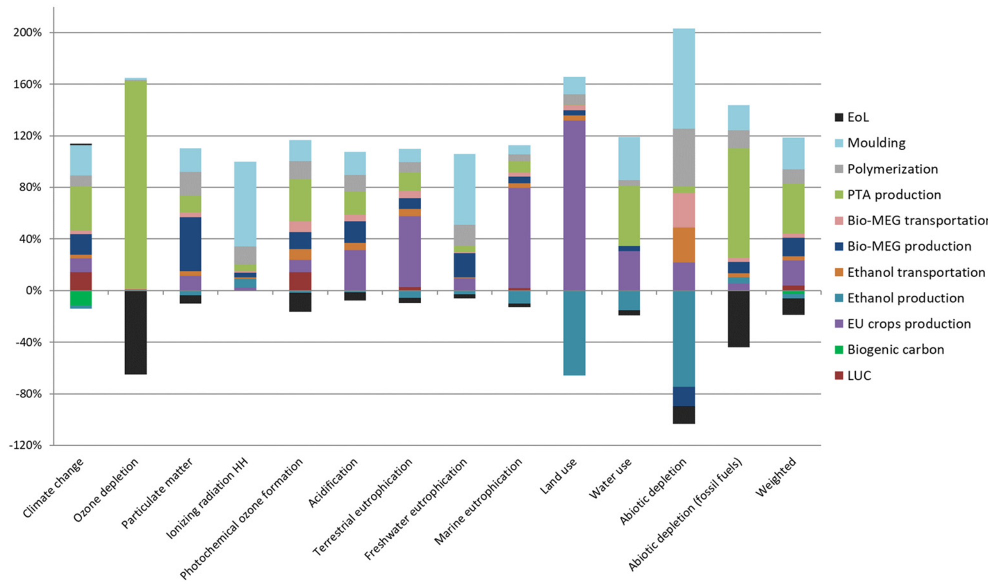

Fig. 5. Breakdown of the cradle-to-grave impact of bio-based PET bottles from European crops (Alternative 1) per functional unit.

the yield of the crop, the lower the LUC impact. The average yield of the EU crops was 11 Mg DM ha^{-1} which is less than the average yield of Brazilian sugarcane (22.7 Mg DM ha^{-1}).

3.3. Bio-based PET bottles from European wheat straw (Alternative 2)

The breakdown of the cradle-to-grave environmental impact of bio-based PET bottles from European wheat straw (alternative 2) per functional unit of 1 kg is shown in Fig. 6 (Table with background values is provided in the supplementary information).

This product system differs from the baseline only for the wheat straw and ethanol production unit processes. Except for abiotic depletion, where it represents 19% of the impact, wheat straw generates a negligible contribution to the cradle-to-grave impacts. Wheat straw is a residue and has no LUC impacts, since LUC should be assigned only to wheat grains which are the market driver of wheat cultivation. The consequence of removing wheat straw from the field is modelled by accounting for the marginal N, P and K mineral fertilizers that need to be applied. These are the cause of the impacts for abiotic depletion. The ethanol production process does not show significant contribution in any impact categories (maximum 6%). The main reason is that the energy requirements are satisfied internally by burning lignin, which is a by-product of the process itself.

3.4. Comparison of cradle-to-grave environmental impacts of PET bottles

Fig. 7 shows the comparison of the cradle-to-grave environmental impacts of the investigated product systems. As explained in Section 2.1.4, only 8 impact categories were considered suitable for comparison with petrochemical PET bottles.

For all product systems, PTA production, polymerisation, moulding and EoL processes are identical. The difference in impacts between

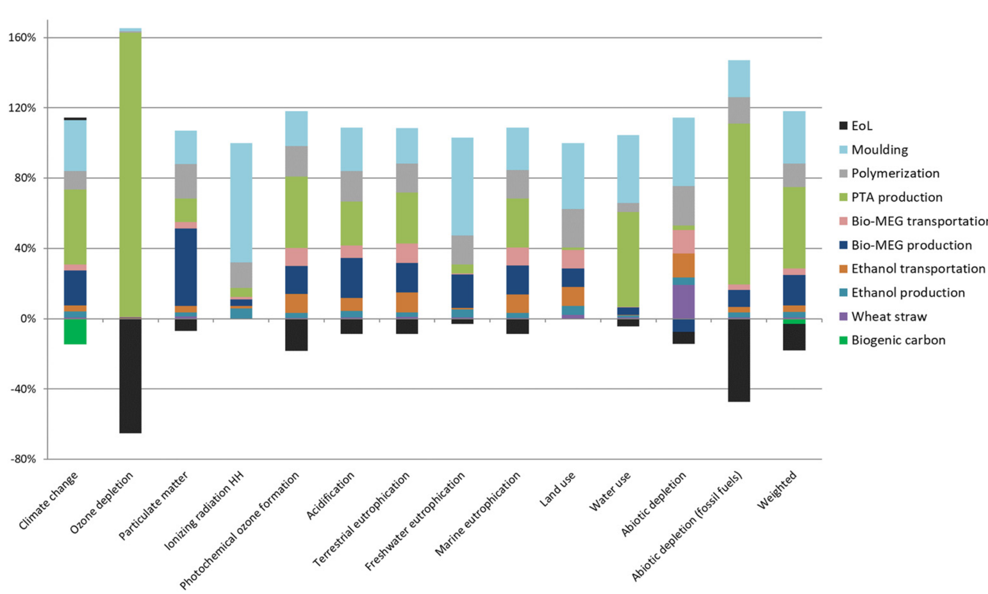

Fig. 6. Breakdown of the cradle-to-grave impact of bio-based PET bottles from wheat straw (Alternative 2) per functional unit.

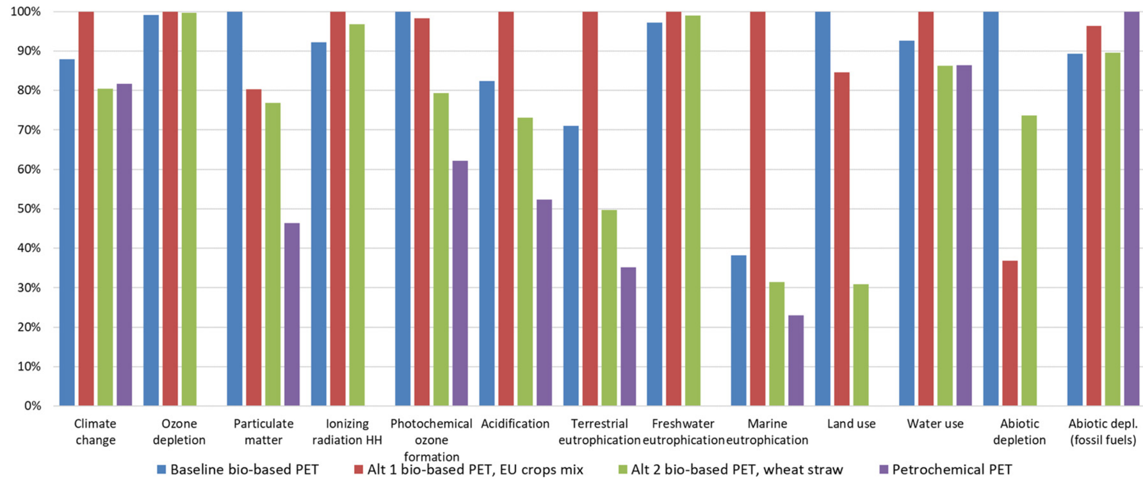

Fig. 7. Comparison of the cradle-to-grave impact of bio-based and petrochemical PET bottles per functional unit. For better visualization, the value of 100% was assigned to the highest impact among the product systems investigated.

petrochemical and bio-based PET bottles lies in how bio- or fossil-based MEG is produced. For the bio-based product systems, the feedstocks used in the production of ethanol (Brazilian sugarcane, EU crops or wheat straw) varies which results in differences in the associated biomass production, ethanol production and LUC impacts.

Among the bio-based product systems, the bio-based PET bottles from straw (alternative 2) perform the best overall. The bio-based PET bottles derived from EU crops (alternative 1) performs the worst in almost all categories except for the particulate matter, photochemical ozone formation, land use and abiotic depletion impact categories where the baseline bio-based PET bottles perform the worst. The alternative 1 product system shows lower impacts for land use and abiotic depletion categories due to the avoidance of animal feed production with the DDGS by-product (and subsequent avoided use of fertilizers to produce feed). However, for acidification, terrestrial and marine eutrophication, they perform worse arising from the use of fertilizers and lower yields attained than Brazilian sugarcane.

When comparing bio-based PET bottles with petrochemical PET bottles, petrochemical PET bottles show overall lower impacts. The difference is reduced (0–15%) when straw is used as feedstock (alternative 2). Among the impact categories considered suitable for comparison, petrochemical PET bottles perform the worst only in the abiotic depletion of fossil fuels category. Using bio-based PET bottles to replace petrochemical PET bottles show the possibility to lower fossil fuel depletion up to 11%. For climate change, bio-based PET bottles from straw (Alternative 2) have the best performance with petrochemical PET bottles showing a similar performance (2% variation). Bio-based PET bottles derived from EU crops shows the worst performance with about 18% higher GHG emissions compared to petrochemical PET bottles. While for baseline bio-based PET bottles the difference is 7%. If the LUC impacts are not considered, the difference drops to 2%.

4. Discussion

Overall, the results show that for bio-based PET to be preferable to fossil-based PET, further improvement regard to its environmental performance is needed. This is in line with the findings of previous LCA studies on bio-based PET bottles, even though they have differences in several LCA methodology aspects (Benavides et al., 2018; Chen et al., 2016; Tsiropoulos et al., 2015). For partially bio-based PET bottle cases, the studies report a comparable GHG emission performance to fossil-based PET bottles (mostly in the range of $\pm$10%) and a favourable performance for fossil fuel consumption compared to fossil-based (reduction of 3–30%). However, the studies that include other impact categories (e.g. acidification, terrestrial eutrophication, particulate matter) show bio-based PET bottles to have a worse performance compared to PET bottles mostly in relation to the fertilizer application, and chemicals and energy demands in processing, which is paralleled in this study (Chen et al., 2016). The reader can refer to a recent review paper by Walker and Rothman for an overview of LCA results and the variation that exists between previous LCA studies comparing bio-based and petrochemical plastics (Walker and Rothman, 2020). Tsiropoulos et al. consider improvement potentials for bio-MEG process by having a CHP plant, process heat integration and more advanced MEG production technology which are estimated to provide up to 20% reduction in GHG emissions (Tsiropoulos et al., 2015) .

Especially for bio-MEG production, process energy requirements, which are met by coal-based steam and grid electricity showed significant contribution to environmental impacts in several impact categories. This is due to availability of coal in India and thereby its use as a primary fuel for energy production. A fuel switch from coal to natural gas or biomass for generation of energy used in bio-MEG production would result in reduction of impacts (estimated above 10% reduction of GHG emissions) and improve the overall performance of bio-based PET bottles.

Looking at options to drastically improve the performance of bio-based PET in the future, one would be to increase the efficiency of bio-MEG production. The commercial bio-MEG production described in this article follows a multi-step route (via ethanol, ethylene, ethylene oxide) with a low overall efficiency. There are currently direct routes from sugars to bio-MEG being developed by several companies (i.e. Avantium, HaldorTopsoe/Braskem, UPM, ENI Versalis) and tested to bring to commercial scale (Avantium, 2019a; de Jong et al., 2020). Another option is making the PTA component from biomass. There are ongoing studies examining different routes to bio PTA (Collias et al., 2014; Volanti et al., 2019), but still it seems a long way before they will be cost competitive with fossil based PTA. Instead, several companies including Avantium and Corbion Purac are working on processes for commercially viable production of 2,5-Furandicarboxylic acid (FDCA) as a potential bio-based replacement for PTA (Avantium, 2019b). This is used together with bio-MEG in the production of polyethylene furanoate (PEF), a new polymer that is 100% bio-based, expected to enter the market in 2023 with similar (or superior) properties to PET (Skoczinski et al., 2021).

The effects of land-use changes were considered in this study. However, there is still no consensus on the method for calculating the ILUC emissions and therefore PEFCR guidance excludes the ILUC impacts. A deterministic approach based on historical deforestation data (2000

−2010) was developed within this study, building on the approaches recently presented by (Tonini et al., 2016). As it builds upon historic data, the method does not estimate the impacts of the future cropland demand for EU bio-based products but provides an estimate of the overall deforestation and intensification emissions associated with one hectare of cropland in the past. The modelling of indirect effects is so far limited to GHG emissions. We recommend that this needs to be extended to other impact categories. The LUC approach we used allows to reflect on impacts caused in all environmental impact categories.

In the EoL modelling, several uncertainties exist. Bio-based PET bottles are chemically identical with petrochemical counterparts which allows the use of existing data for waste management of petrochemical PET bottles for modelling the impacts. Yet, there is high variability in collection and sorting efficiency between European countries due to the fact that PET beverage bottles in some European countries are part of a refund system. This differs from the ordinary heterogeneous plastic waste stream collected in households, where the quality is much lower. Therefore, there could be variation in the contribution of EoL options where increase in contribution of recycling is favoured for improved environmental performance. This is also expected with the policy ambition of EU to increase recycling rates (European Commission, 2018a). Furthermore, concerning the assessment of landfilling impacts with LCA can result in contradictory results with the waste hierarchy (that considers landfilling as the least preferable EoL option). From a climate impact perspective, non-biodegradable (bio-) plastics that lock away carbon for long time periods might actually show positive impacts. However, climate change is not the only challenge, and the ecosystem damages caused by landfilling need to be understood especially for non-degradable and persistent products.

Littering is a central issue in public discussion about plastic items. Nevertheless, littering is not included in this LCA due to lack of data and a missing assessment methodology to assess such phenomenon. Fate, exposure, and effect modelling for macro- and micro-plastics is still in its infancy. Physical impacts (e.g. entanglement; ingestion of larger plastic particles and their effects), chemical impacts (e.g. due to microplastic formation, microplastics as carriers of other chemicals, unknown impact of additives) and biological impacts (e.g. microplastics as carriers of germs/alien species) are largely unknown. We recommend further research on this topic (inventory data collection as well as impact assessment method development) to be able to take into account the associated impacts of littering (e.g. leaving plastics in the soil or in a marine environment). One project currently running is MaRILCA looking at integrating potential environmental impacts of marine litter into LCA (MarILCA, 2020).

The current availability and transparency of data for petrochemical PET hampered the comparison with bio-based PET bottles that should consider more categories to provide a broader environmental comparison. It would be recommended to have more transparent datasets in the public domain (e.g. by PlasticsEurope and the LCI data owners). Only by this way it is possible to make the comparison with full insights over all impact categories and have a full interpretation of the results with the ability to trace back to the activity level data.

5. Conclusions

This study provides important insights in the interest of the EU policy audience because scientific information is requested as support for future bioeconomy and plastic strategies. The cradle-to-grave environmental performance of bio-based PET bottles (with about 30% bio content) were compared with petrochemical PET bottles. A comprehensive assessment was performed using thirteen impact categories following PEF methodology and including the impacts of land-use change and end-of-life representing current European practice.

PTA production and stretch blow moulding processes, which are the same for bio-based and petrochemical PET bottles, were found as the highest contributors to the overall weighted environmental impacts of bio-based PET bottles (about 39–46% for PTA production, 25–30% for moulding). However, the impacts of production of biomass are highly prominent in land use as well as terrestrial eutrophication due to fertilizer application. The EoL stage has a relatively low relevance (about 10% on weighted bases). It provides an overall credit owing to the substitution of virgin plastic impacts by recycling and substitution of heat and electricity with incineration. The impact of land use change was also considered in this study which is relevant for the sugarcane and the EU crops cultivation. LUC impact was found to be minor (2–4% on weighted bases). Only for climate change and photochemical ozone both categories, LUC impacts were considerable (6–14% contribution to cradle to grave results).

Baseline bio-based PET bottles performed worse compared to conventional petrochemical PET bottles in most impact categories. They offer very minor environmental benefits compared to petrochemical PET bottles i.e. a slight impact reduction (about 10%) in abiotic depletion (fossil fuels). Comparable performance is observed for climate change (less than 2% difference without the impacts from LUC, and 7% with LUC). Using European crops for ethanol production instead of Brazilian sugarcane (alternative 1) resulted in overall lower performance due to the lower yields attained than Brazilian sugarcane. Lower yields lead to use of more resources and utilities such as water, fertilizer, pesticides as well as higher direct energy requirements and direct emissions for the production of same amount of product. The impact of bio-based PET bottles became close to (but not better than) that of petrochemical PET bottles when wheat straw was considered as biomass feedstock for ethanol production (alternative 2).

Overall, the results show that to make bio-based PET preferential in terms of sustainability performance differences in production are needed (e.g. shift in source of fuel used for energy, switch to a direct route for MEG production).

CRediT authorship contribution statement

Iris Vural Gursel: Conceptualization, Methodology, Software, Data curation, Formal analysis, Investigation, Visualization, Writing – original draft, Writing – review & editing. **Christian Moretti:** Visualization, Writing – original draft, Writing – review & editing. **Lorie Hamelin:** Methodology, Data curation, Formal analysis, Writing – review & editing. **Line Geest Jakobsen:** Methodology, Data curation, Software, Formal analysis, Writing – original draft. **Maria Magnea Steingrimsdottir:** Methodology, Data curation, Software, Formal analysis, Writing – original draft. **Martin Junginger:** Supervision, Funding acquisition, Resources, Writing – review & editing. **Linda Høibye:** Project administration, Funding acquisition. **Li Shen:** Conceptualization, Methodology, Project administration, Funding acquisition, Resources, Supervision, Writing – review & editing.

Declaration of competing interest

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

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Appendix A. Impact categories

Table A1 provides the 13 impact categories considered and their assessment methods. Only the impact assessment methods for land transformation and particulate matter were based on the EU PEF guide (Manfredi et al., 2012) due to insufficient inventory details to properly assess these two categories with the methods recommended by the PEFCR guidance. Normalization and weighting factors are presented in the same table. Such factors were used in identifying the most relevant unit processes and impact categories (that contribute the most to the total normalized and weighted environmental impacts) for each product system. Table A1 also indicates the eight impact categories that were found suitable to be used for the comparison with petrochemical PET bottles. Further information provided in Section 2.1.4.

Table A.1
Impact categories considered, their assessment methods, normalization and weighting factors. In the last column, X denotes the impact categories found suitable for the comparison with petrochemical PET bottles.

Impact category	Unit	Assessment method	Normalization factors EU 27 per person (Benini et al., 2014; European Commission, 2018b)	Weighting factors without toxicity (Benini et al., 2014; European Commission, 2018b)	Comparison with petrochemical PET
Climate change	kg CO_2eq	IPCC, 2013 GWP 100a (IPCC, 2013)	9.22E+03	22.19	X
Ozone depletion	kg CFC-11 eq	(Ramanathan and Feng, 2009)	2.16E-02	6.75	
Particulate matter	kg PM2.5 eq	(Rabl et al., 2014)	3.80E+00	9.54	X
Ionizing radiation Human Health (HH)	kBq U^{235} eq	(Frischknecht et al., 2000)	1.13E+03	5.37	
Photochemical ozone formation	kg NMVOC eq	(van Zelm et al., 2008)	3.17E+01	5.1	X
Acidification	mol H+ eq	(Posch et al., 2008)	4.73E+01	6.64	X
Terrestrial eutrophication	mol N eq	(Posch et al., 2008)	1.76E+02	3.91	X
Freshwater eutrophication	kg P eq	(Goedkoop et al., 2009)	1.48E+00	2.95	
Marine eutrophication	kg N eq	(Goedkoop et al., 2009)	1.69E+01	3.12	X
Land transformation	kg C deficit	Soil Organic Matter (Milà i Canals et al., 2007)	7.48E+04	8.42	
Water use	m^3	AWARE (Boulay et al., 2015)	1.15E+04	9.03	X
Abiotic depletion	kg Sb eq	(van Oers et al., 2002)	5.79E-02	8.08	
Abiotic depletion (fossil fuels)	MJ	(van Oers et al., 2002)	6.53E+04	8.92	X

Appendix B. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2021.148642.

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