



An Eco-profile and Environmental Product Declaration of the PET Manufacturers in Europe

Polyethylene Terephthalate (PET) (Bottle Grade)

CPME

June 2017



Introduction

This Environmental Product Declaration (EPD) is based upon life cycle inventory (LCI) data from PlasticsEurope's Eco-profile programme. It has been prepared according to **PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology and PCR for Uncompounded Polymer Resins and Reactive Polymer Precursors**

[PlasticsEurope, 2011a]. EPDs provide environmental performance data, but no information on the economic and social aspects that would be necessary for a complete sustainability assessment. Further, they do not imply a value judgment between environmental criteria.

This EPD describes the production of bottle grade polyethylene terephthalate (PET) from cradle to gate (from crude oil extraction to PET granulate at plant). **Please keep in mind that comparisons cannot be made on the level of the polymer or the polymer precursor alone:** it is necessary to consider the full life cycle of an application in order to compare the environmental performance of different materials and the effects of relevant processes during the whole life cycle. This EPD is intended to be used by member companies, to support product-orientated environmental management; by users of plastics, as a building block of life cycle assessment (LCA) studies of individual products; and by other interested parties, as a source of life cycle information.

Meta Data

Data Owner	CPME aisbl
LCA Practitioner	IFEU Heidelberg, Germany
Programme Owner	PlasticsEurope aisbl
Programme Manager, Reviewer	Schulz Sustainability Consulting on behalf of DEKRA Assurance Services GmbH
Number of plants included in data collection	12

Representativeness	Good (85 % of installed production capacity covered)
Reference year	2015
Year of data collection and calculation	2016
Expected temporal validity	2020
Cut-offs	none
Data Quality	good
Allocation method	physical

Description of the Product and the Production Process

This EPD represents the average industrial production of PET in Europe from cradle to gate.

Production Process

PET production covered by this study is by esterification of ethylene glycol and terephthalic acid (PTA). The esterification process is carried out under moderate pressure (2.5-5.5 bar) and at high temperature (230-270 °C) whilst the water formed during the reaction is continuously removed via distillation.

In addition to these foreground processes, the following processes in the supply chain are considered: extraction and refinery of crude oil and natural gas, steam cracking of hydrocarbons (predominantly naphtha) into lower olefins and pygas, catalytic reforming of naphtha, and the extraction and production of p-xylene from both pygas and reformat (xylene loop) production of purified terephthalic acid (PTA) and production of ethylene glycol (MEG). Furthermore, all processes related to the production of electric and thermal energy including their upstream processes are considered as well as the treatment of wastes.

Impacts related to abnormal process conditions (e.g. accidents) are not considered in the present study.

Data Sources and Allocation

Confidential input and output data for the PET production processes including on-site energy production was provided by 7 European PET producers for 12 production plants (primary data).

Data concerning the upstream processes PTA production, steam cracking, catalytic reforming, fossil fuels extraction and refinery were taken from the Eco-profiles of purified terephthalic acid [CPME, 2016] and steam cracker products [PlasticsEurope, 2012]. Country specific electricity mixes were used for grid electricity supply. On-site production of electricity and steam was partially modelled using primary data from the PET producers; data gaps in on-site energy production were closed using European average data of power plants and steam boilers. Representative literature data and the database Ecoinvent v3.3 have been used to fill gaps where no primary data was available and to crosscheck primary data.

Within the foreground system economic allocation was applied for off-spec PET (<0.2 % of total PET output). Concerning the background processes, allocation was intended to be avoided; where necessary, processes have been allocated by physical properties, such as mass, energy, or enthalpy.

Use Phase and End-of-Life Management

The use phase and end-of-life processes of the investigated polymer precursor are outside the system boundaries of the cradle-to-gate system covered by the present study: the major object is the analysis of PET production, which is used in a broad range of applications. However, the treatment of waste from production processes is considered within the system boundaries of this Eco-profile.

Environmental Performance

The tables below show the environmental performance indicators associated with the production of 1 kg of PET. **Due to changes in datasets and methodology a direct comparison of the current Eco-profile results with the previous ones (published in 2011) is not possible!** Please refer to the full Eco-profile report for details.

Input Parameters

Indicator	Unit	Value
Non-renewable energy resources ¹⁾	MJ	69.6
• Fuel energy	MJ	35.5
• Feedstock energy	MJ	34.1
Renewable energy resources (biomass) ¹⁾	MJ	1.6
• Fuel energy	MJ	1.6
• Feedstock energy	MJ	0.0
Abiotic Depletion Potential		
• Elements	kg Sb eq	2.41E-04
• Fossil fuels	MJ	62.0
Water use	kg	95.8
• for process	kg	6.7
• for cooling	kg	89.0
Water consumption	kg	48.8

¹⁾ Calculated as upper heating value (UHV)

Output Parameters

Indicator	Unit	Value
Global Warming Potential (GWP)	kg CO ₂ eq	2.19
Ozone Depletion Potential (ODP)	g CFC-11 eq	0.018
Acidification Potential (AP)	g SO ₂ eq	6.47
Photochemical Ozone Creation Potential (POCP)	g Ethene eq	2.31 ³⁾
Eutrophication Potential (EP)	g PO ₄ eq	1.49
Dust/particulate matter (≤ 10 μm) ²⁾	g PM10	5.64
Total particulate matter ²⁾	g	5.94
Waste	g	9.1
• Non-hazardous	g	8.8
• Hazardous	g	0.3
• Unspecified	g	0.0

²⁾ Including secondary PM10

³⁾ Including NMVOC (1.80 g Ethene eq./kg PET)

Additional Environmental and Health Information

CPME has continued to fully support initiatives to improve the safety and environmental performance of PET production. Changes in production methods have led to near zero human exposure to process chemicals. The environmentally sound treatment of process effluents is being continuously upgraded and now represents the best available technology.

Additional Technical Information

Production technology of PET and its precursors is constantly improved. New production processes and catalyst recovery methods lead to better products quality produced in a more efficient way. Advanced European PET products meet all of the strict existing and upcoming regulatory requirements particularly for food contact applications such as beverage bottles.

Additional Economic Information

Constant product and process innovation of PET has led to energy savings in production, transportation and use of resources. PET is a globally traded commodity and the European PET production facilities provide essential support to local and European economy and can theoretically meet 100% of European demand; the import quota of PET is currently at 20%.

Information

Data Owner

Committee of PET Manufacturers in Europe (CPME aisbl)

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Programme Manager & Reviewer

DEKRA Assurance Services GmbH This Environmental Product Declaration has been reviewed by DEKRA Assurance Services GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006.
Registration number: PlasticsEurope 2016-003, validation expires on 30 November 2018 (date of next revalidation review).

Programme Owner

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For copies of this Eco-Profile, for the underlying LCI data (Eco-profile); and for additional information, please refer to <http://www.plasticseurope.org/>.

References

PlasticsEurope 2011: Eco-profiles and environmental declarations – LCI methodology and PCR for uncompounded polymer resins and reactive polymer precursor (version 2.0, April 2011).

PlasticsEurope 2012: Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers - Ethylene, Propylene, Butadiene, Pyrolysis Gasoline, Ethylene Oxide (EO), Ethylene Glycols (MEG, DEG, TEG), November 2012.

CPME 2016: Eco-profiles and Environmental Product Declarations of the PET Manufacturers in Europe - Purified Terephthalic Acid (PTA). CPME, February 2016



Goal & Scope

General

The Association of Plastics Manufacturers in Europe (PlasticsEurope) has a long tradition of reporting product related environmental data to the public. The PlasticsEurope data sets have become a widely used information basis for all LCA practitioners who are confronted with tasks that included plastic products.

Since permanent technological progress is made also the basic input-output data of the processes involved to produce a plastic product is changing. Constant environmental improvement of production related resource use and emissions is happening as well as the auxiliary processes such as transportation and energy generation are also in continuous development. Accordingly, a regular update of the basic datasets is necessary.

The PET Eco-profile available at the PlasticsEurope webpage was last calculated in 2011. As PET production technology has changed in the last ten years along with the dynamic market for PET bottles, CPME commissioned IFEU to update the Eco-profile for bottle grade Polyethylene Terephthalate (PET).

Intended Use & Target Audience

Eco-profiles (LCIs) and EPDs from this programme are intended to be used as »cradle-to-gate« building blocks of life cycle assessment (LCA) studies of defined applications or products. LCA studies considering the full life cycle (»cradle-to-grave«) of an application or product allow for comparative assertions to be derived. It is essential to note that comparisons cannot be made at the level of the polymer or its precursors. In order to compare the performance of different materials, the whole life cycle and the effects of relevant life cycle parameters must be considered.

This Eco-profile and EPD represents a polymer precursor production system with a defined output. It can be used as modular building block in LCA studies. However, this integrated industrial system cannot be disaggregated further into single unit processes, because this would neglect the interdependence of the elements, e.g. the internal recycling of feedstocks and precursors between different sections of integrated production sites.

This Eco-profile and EPD is prepared in accordance with the stringent ISO 14040–44 requirements. Since the system boundary is »cradle-to-gate« its reference flows are disparate and refer to a broad variety of polymers and precursors. Therefore in accordance with ISO 14040–44, a direct comparison of Eco-profiles is not possible. Whilst ISO 14025, Clause 5.2.2 does allow EPDs to be used in comparison, PlasticsEurope EPDs are derived from Eco-profiles, i.e. with the same »cradle-to-gate« system boundaries.

As a consequence, a direct comparison of Eco-profiles or EPDs makes no sense because 1 kg of different polymers are not functionally equivalent.

Once a full life cycle model for a defined polymer application among several functionally equivalent systems is established, and only then, can comparative assertions be derived. This principle applies also to EPDs, for instance, of products where PlasticsEurope derived EPDs can serve as building blocks.

Eco-profiles and EPDs are intended for use by the following target audiences:

- Member companies, to support product-orientated environmental management and continuous improvement of production processes (benchmarking);
- Downstream users of plastics precursors and plastics, as a building block of life cycle assessment (LCA) studies of plastics applications and products; and
- Other interested parties, as a source of life cycle information.

Product Category and Declared Unit

Product Category

The core product category is defined as **uncompounded polymer resins, or reactive polymer precursors**. This product category is defined »at gate« of the polymer or precursor production and is thus fully within the scope of CPME as the representative industry association.

Functional Unit and Declared Unit

The Functional Unit and Declared Unit of the PET Eco-profile is:

1 kg of primary uncompounded PET (bottle grade) »at gate« (production site output) representing a European industry production average.

Product and Producer Description

Properties of PET

PET is a thermoplastic polyester with the CAS number 25038-59-9 and a gross calorific value of 24 MJ/kg. The structural formula of PET is shown in Figure 1. The most important application fields of PET are fibres, films and bottles. Every end-use requires specific properties – thus different PET grades exist for fibres, films and bottles. In this context, the most important consideration is the molecular weight of the polymer, which is usually reported as intrinsic viscosity (I.V.). In this Eco-profile only bottle grade PET is considered. The requirements for this grade are high I.V. from 0.7 – 0.85 dL/g.

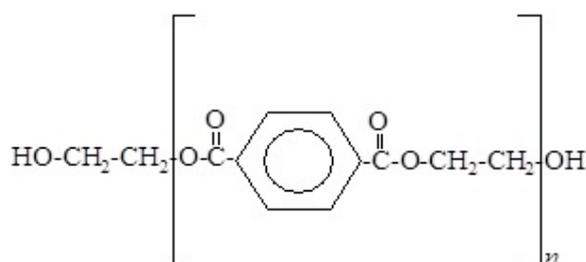
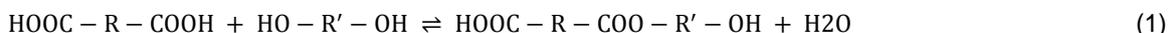


Figure 1: The structure of polyethylene terephthalate. The unit inside the brackets will typically have a repeat value (n) in the range 100 to 200.

Such condensation polymers are typically produced by reaction of compounds containing two carboxyl groups (-COOH) with compounds containing two alcohol groups (-OH) according to a general reaction as follows:

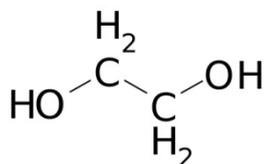


where R and R' represent organic groups. The ester in reaction (1) may now react with further acid or alcohol to produce a long chain polymer.

For PET, the acid component used is terephthalic acid:



and the alcohol component is ethylene glycol (ethane-1,2-diol):



The commercial production of PET

A process flowchart as an overview of the processes required for PET production is given in Figure 3: . The monomers of PET production, purified terephthalic acid (PTA) and mono ethylene glycol (MEG) are polymerised in the liquid phase to produce amorphous PET. This form of the polymer is suitable for the production of fibres and film. Most bottle grade PET today is a copolyester slightly modified through addition of 1-2% Benzene-1,3-dicarboxylic acid (isophthalic acid, IPA) or 4(hydroxymethyl)cyclohexyl-methanol (cyclohexanedimethanol, CHDM) during polymerisation.

The first step of PET production is the esterification of PTA and MEG to bishydroxyethyl terephthalate (BHET) with water as a by-product (see equation (1)) at around 220-260 °C in the presence of an anti-mony catalyst (usually Sb_2O_3). Water forming from the esterification reaction is continuously removed by distillation. Formation of the undesired side product diethylene glycol is suppressed by maintaining low molar ratios of MEG:PTA (less than 2 or even 1.5). BHET is then sent to Pre-polycondensation in a second reactor under a vacuum and further to a melt polycondensation reactor at higher temperatures and still under vacuum. Vacuum is required to remove water and other side products and to drive the reaction equilibrium towards the polymer.

As melt polymerisation does not produce high molecular weight, a subsequent polymerisation step, solid state polymerisation (SSP) is required for bottle grade PET. During SSP the polymer chain lengths are increased by heat in the absence of oxygen and water, by means of either vacuum or purging with an inert gas to drive off the by-products of reactions. The reaction is driven by temperature, pressure, and the diffusion of by-products from the interior of the pellet to the surface. The product of SSP is a partially crystalline resin that can be used to produce bottles via injection moulding and stretch blow moulding.

Upstream Chains

PTA production [CPME, 2016]

Crude terephthalic acid (CTA) is produced by oxidation of p-xylene. A subsequent purification step leads to purified terephthalic acid (PTA). The oxidation reaction is catalysed by cobalt-manganese-bromide catalysts. Acetic acid is used as solvent, and compressed air is used for oxygen supply. As a bromide source, usually hydrobromic acid is used, but sodium bromide (NaBr), tetrabromoethane or other bromide compounds are also possible. The conversion of p-xylene is usually carried out in bubble column reactors in liquid phase at elevated temperature (175-225 °C) and pressure (15-30 bar). From the reactor effluent, crude terephthalic acid (CTA) is obtained by crystallisation and centrifugation/filtration. Vapour output from the reactor is condensed in heat exchangers and the condensate (mostly acetic acid and water) is recycled to the reactor. Steam generated from residual heat of this condensate is usually used internally. Liquid output from the centrifuge/filters is also recycled to the reactor after de-gassing and dehydration. For purification, CTA is entirely dissolved in water (at >260 °C) and brought into contact with hydrogen in the presence of a Pd catalyst. Under these conditions the undesired co-product 4-carboxybenzaldehyde (4-CBA) is converted to p-toluic acid, which is separated from terephthalic acid in a series of crystallisers. After centrifugation/filtration and drying, purified terephthalic acid (PTA) is obtained as powder.

p-xylene production [PlasticsEurope, 2013]

The main source of xylenes in Europe (and the USA) is reformat (86 % in 2012) [European Commission, 2014], a product of catalytic conversion of naphtha. A minor part of European xylene is produced from pyrolysis gasoline, which is a product of thermal cracking of hydrocarbons (steam cracking), also mainly based on naphtha (74 % of the feedstock) regarding European production. Both reformat and pyrolysis gas (which has to be hydrotreated to saturate mono- and diolefins and to remove sulphur compounds) are usually fed to a so-called aromatics complex, where the aromatic feedstock is separated and/or chemically converted into the desired products benzene, toluene, p-xylene, o-xylene, and/or a mixture of xylenes.

In a first step, the feedstock is fractionated in a distillation column into a benzene/toluene cut, which also contains the nonaromatic compounds, and into the higher boiling xylenes (including ethylbenzene and styrene) and higher aromatics fraction. Benzene and toluene are separated from the non-aromatics (raffinate) by solvent extraction (liquid-liquid extraction). Usually, highly polar substances are used as solvents in an extraction column. The paraffinic raffinate from the top of the column is usually fed to the gasoline pool. Aromatics are extracted from the solvent by distillation and stripping. In two further distillation steps benzene and toluene are recovered as pure products. In a transalkylation/disproportionation unit, overhead toluene can be converted into additional xylenes. For transalkylation higher aromatics (e.g. trimethylbenzenes) are co-fed with toluene to produce only xylenes. During disproportionation two toluene molecules react to form one molecule of benzene and xylene, respectively. Typical processes are carried out at temperatures of 260-530 °C and pressures of 2-46 bar on either zeolitic or alumina/silica catalysts.

The xylenes and higher aromatics obtained at the bottom of the feed splitter column together with the xylenes produced in the transalkylation/disproportionation unit are fed to a xylene column. This fractionation unit is designed to either completely separate the xylenes from higher aromatics or to additionally recover a part of o-xylene in the bottoms. In the latter case, o-xylene can be obtained as product after a further distillation step. Higher aromatics (C9+) are either used in toluene transalkylation or blended into

the gasoline pool. The xylenes from the top of the xylene column are fed to the so-called xylene loop, consisting of a p-xylene extraction unit and a xylene isomerisation unit. In the first unit high purity p-xylene is extracted from the equilibrium xylene mixture either by crystallization (-60 to -70 °C, atmospheric pressure) or by adsorptive separation (120-175 °C). The remaining xylene mixture (containing also ethylbenzene and styrene) is fed to an isomerisation unit where a near-equilibrium distribution of xylene isomers is re-established, meaning that new p-xylene is formed from the remaining o- and m-xylenes. The acidic metal-containing zeolite catalyst used here also isomerizes ethylbenzene selectively to xylene isomers in their equilibrium ratio. Hydrogen is added to the isomerisation unit to prevent hydrogenolysis of the aromatics on the metal sites. The mixed xylenes (and by-product C9+-aromatics) are recycled to the xylene column after separation from light by-products (light ends (methane and hydrogen), benzene, toluene) through fractionation, and from unsaturated components by clay treating.

Ethylene oxide and ethylene glycol production [PlasticsEurope, 2012]

The most common way of producing ethylene oxide is by reacting gaseous ethylene and oxygen over an aluminium oxide supported silver catalyst. The exothermic reaction is carried out at elevated temperature (200 to 300 °C) and pressure (15 to 25 bar) with very short residence times (around 1 second). Ethylene glycols (mono ethylene glycol, diethylene glycol, triethylene glycol, and heavier glycols) are formed by the hydrolysis of ethylene oxide with water at elevated temperature and pressure (150 to 250 °C, 30 to 40 bar). In practice most ethylene oxide / ethylene glycol plants are designed as integrated plants for a production mix of high purity ethylene oxide and glycols.

Feedstock ethylene is typically received by pipeline from a steam cracker. Oxygen is usually provided in pure form by pipeline from an air separation unit. The reaction between ethylene and oxygen is carried out in a multi-tubular fixed bed type reactor containing the catalyst particles (spheres or rings with 3-8 mm diameter) inside the tubes and a coolant on the shell side. The heat generated by the exothermic reactions is removed by the coolant, and is recovered by means of steam production. The steam is used as a heating medium in various sections of the plant.

Due to various reasons (e.g. flammability of ethylene oxide and ethylene, temperature control of the reactor, high ethylene oxide selectivity only achievable at low ethylene conversion), low ethylene feed concentrations (15-40 vol %) and low ethylene conversions (7-15 %) are reasonable. Thus, a large gas flow is circulated continuously through the ethylene oxide reactor. The reaction products ethylene oxide, carbon dioxide and water are removed from the circulating gas while unconverted oxygen and ethylene are recycled back to the reactor.

A mixture of ethylene oxide and water is fed to the glycol reactor which is operated at typical temperatures between 150 and 250 °C. Under these conditions reaction rates are fast and no catalyst is required. Residence time is adjusted to provide total conversion of ethylene oxide. At a reactor pressure of 30 to 40 bar vaporisation of ethylene oxide is avoided. The reactor feed contains an excess of water in order to limit the adiabatic temperature rise and to enhance the selectivity to mono ethylene glycol. Typically the produced glycol mixture consists of 70 to 95 % w/w mono ethylene glycol; the rest consists mostly of diethylene glycol and small quantities of triethylene glycol.

Upstream Processes Oil Refinery and Steam Cracking [PlasticsEurope, 2012]

Petroleum refineries are complex plants in which the combination and sequence of processes are usually very specific to the characteristics of the raw materials, i.e. the composition of the crude oil, and the products to be produced. Refineries are not only different regarding their configuration, process integra-

tion, feedstock, product mix, unit size design and control systems. Differences in market situation, location and age of the refinery environmental regulation are amongst other reasons for a wide variety of refinery concepts. In spite of the large variety of possible and actual refinery configurations, the Draft Reference Document on Best Available Techniques for Mineral Oil and Gas Refineries [European Commission, 2015] describes in its Annex II four typical refinery configurations – from a simple hydro-skimming unit up to a complex refinery with hydro-conversion and a hydro-cracker and/or an Integrated Gasification Combined Cycle Unit (IGCC). The refinery model used for the calculation of the current Eco-profile is a model that represents all typical processes of the different refinery configurations. It considers the capacity weighted mixture of refinery configurations in Europe according to European Commission 2015 and Eurostat, taking the changed product mix in recent years in account. This detailed model comprises the single processes of a petroleum refinery and makes up an average model of the European refinery.

The chemical reaction for the steam cracking process is a dehydrogenation and can be affected either catalytically or thermally. In the European Union the steam cracking process, where the reaction is carried out in the presence of steam and at temperatures of up to 875 °C, accounts for the lion's share of the ethylene, propylene, and butadiene production. Due to the rising demand for ethylene and propylene as precursors for the polymer production not only naphtha, but also gas fractions are used as feedstock for steam cracking. Regardless of feedstock or contractor a cracker complex may be separated into three sections namely pyrolysis, primary fractionation/compression and product fractionation. In the pyrolysis section the hydrocarbon feedstock is preheated and then vaporised with superheated steam before passing into long and narrow tubes arranged in a cracking furnace. In this reactor, the hydrocarbon feedstock is cracked into smaller molecules. The product distribution of the product can be controlled through variation of residence time, temperature profile, and partial pressure. This process is highly endothermic and therefore requires high energy input. Therefore the tubes of the furnace are heated to 750 – 875 °C by oil or gas fire burners. The primary fractionation and compression section consists of the primary fractionator (naphtha and gas oil feed only), quench tower, gas compressor and gas clean-up facilities. The primary fractionator is used to condense and fractionate fuel oil streams produced from naphtha and gas oil fed crackers. The gases are de-superheated in the quench tower by a circulating oil or water stream. The circulating oil or water stream is used as a medium level heat source for the rest of the plant. In the product fractionation section products are cooled down and subsequently fractionated. The chilling train usually consists of four or five successive stages of chilling, incorporating ethylene and propylene refrigeration as well as an elaborate self-refrigeration system.

Upstream Chains of Crude Oil and Natural Gas

The upstream chains of crude oil and natural gas from the Ecoinvent database v3.3 [Ecoinvent, 2016] were used and updated with current primary data from the oil and gas producing industry. Furthermore, upstream chains for natural gas liquids (NGL) and ethane from North Sea fields were derived subsequently. Non-conventional methods for crude oil and natural gas extraction (shale gas, fracking, etc.) were not considered since these techniques were not applied in the countries supplying the EU27 region in the reference year.

Producer Description

This Eco-profile represents European industry averages within the scope of PlasticsEurope as the issuing trade federation. Hence it is not attributed to any single producer, but rather to the European plastics industry as represented by PlasticsEurope's membership and the production sites participating in the Eco-profile data collection. The following companies were contributing data to this Eco-profile:

- Equipolymers GmbH, Germany
- Indorama Ventures Química S.L.U., Spain
- Indorama Ventures Europe B.V., The Netherlands
- Indorama Ventures Poland Sp. z o.o., Poland
- JBF Global Europe BVBA, Belgium
- Lotte Chemical UK Ltd, United Kingdom
- NOVAPET S.A., Spain
- Plastiverd, Pet Reciclado S.A., Spain
- UAB "NEO GROUP", Lithuania
- UAB Orion Global Pet, Lithuania

System description

System Boundaries

General Considerations

The Eco-profile refers to the **production of primary bottle grade PET resin** and is based on a **cradle-to-gate system** (Figure 2). The production stage covers all life cycle processes from extraction of natural resources, up to the point where the product is ready for transportation to the customer. Packaging of the material is not included. In this cradle-to-gate information module, the subsequent steps of conversion, use phase and end-of-life management are not included.

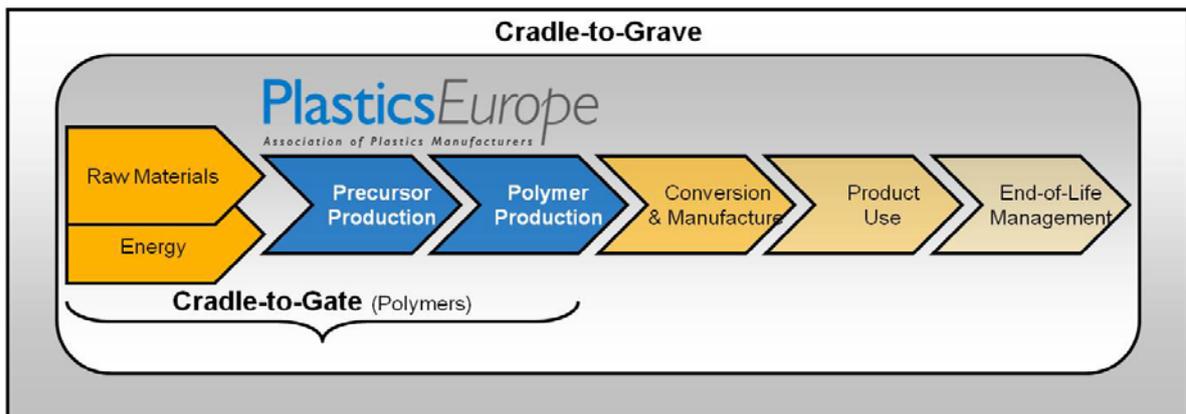


Figure 2: Cradle-to-gate system boundaries.

Cradle-to-Gate System Boundaries for Production

The following processes are included in the cradle-to-gate LCI system boundaries (see also Figure 3):

- Extraction of non-renewable resources (e.g. of oil and natural gas)
- Growing and harvesting of renewable resources (e.g. biomass production)
- Beneficiation or refining, transfer and storage of extracted or harvested resources into feedstock for production;
- Recycling of waste or secondary materials for use in production
- Converting of non-renewable or renewable resources or waste into thermal or electric energy
- Production processes
- All relevant transportation processes (transport of materials, fuels and intermediate products at all stages)
- Management of relevant waste streams or pollution generated by processes within the system boundaries.

According to the methodology of Eco-profiles [PlasticsEurope, 2011a] capital goods, i.e. the construction of plant and equipment as well as the maintenance of plants, vehicles and machinery is outside the LCI system boundaries. The end-of-life treatment of the polymer precursors and their resulting products is also outside the LCI system boundaries of this Eco-profile. Inputs and outputs of secondary materials and wastes for recovery or disposal are noted as crossing the system boundaries without any environ-

mental burdens. An exception is low radioactive waste from electricity generation for which a final storage has not been found yet; it is declared as output.

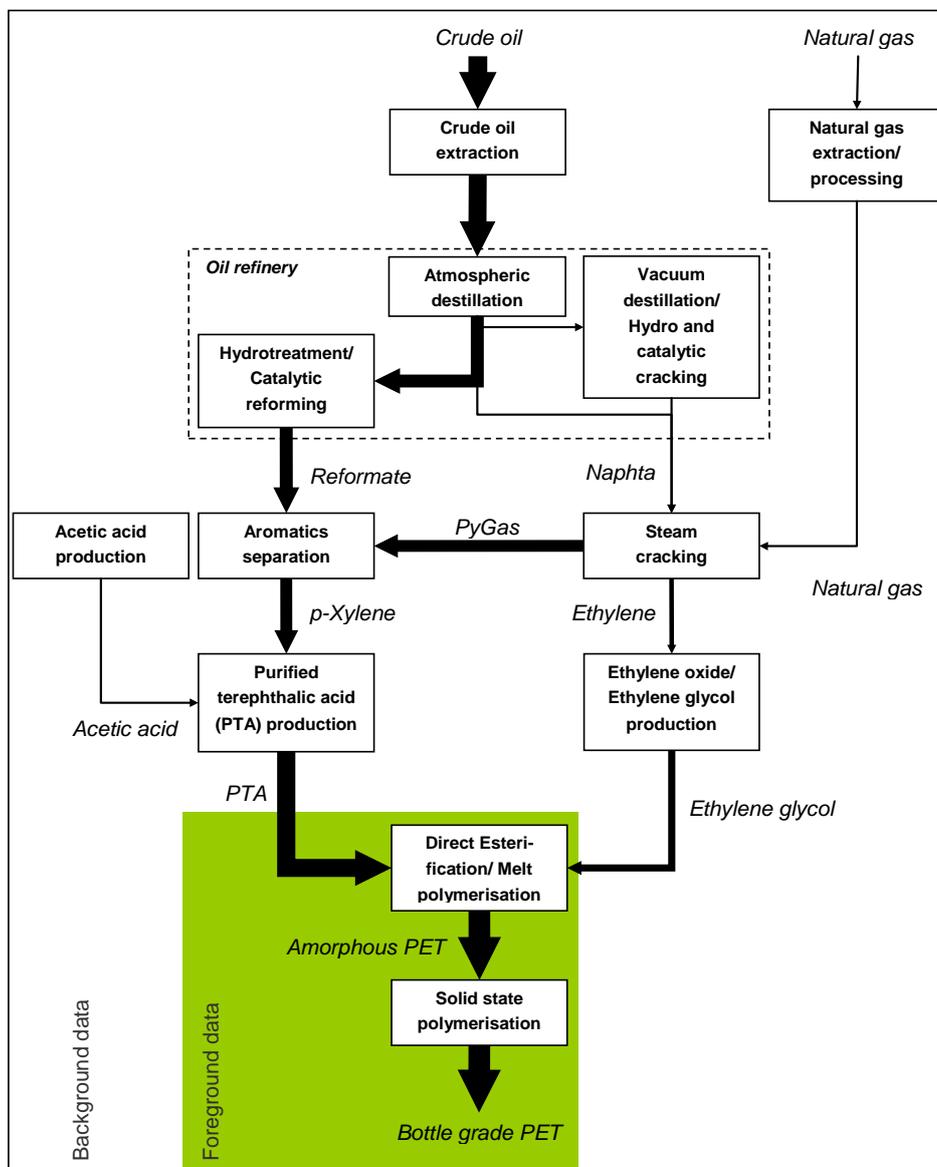


Figure 3: Schematic flow chart of the PET production system

Technological Reference

The LCI data in this Eco-profile represent the average applied technology for the production of PET (bottle grade) in Europe. They are based on confidential data collected from PET production sites. Thus, primary data were used for all foreground processes (under operational control) as well as for the provision of on-site energy, if applicable. These input data are complemented with secondary data from background processes, e.g. grid electricity supply and the raw material pre-chain. PET production from secondary material (PET waste) and PET imported to Europe are not considered in this Eco-profile as this was outside the scope of this project.

Temporal Reference

The LCI data for production were collected as sum over 12 months representing an annual average, to compensate for any seasonal fluctuations of input data. Data was provided for the year 2015. Thus, the reference year for this Eco-profile is 2015 with a maximum temporal validity until 2020. It can be assumed that the growth and consolidation phase will continue in the next years. Thus, it seems adequate to refer to the 5-year interval that was proposed in the Product Category Rules for Polymers [PlasticsEurope, 2011a]. The data describing the PTA production and the connected upstream processes were taken from the PTA eco-profile stating 2011-2013 as the reference time period. MEG production data refers to the year 2009 [PlasticsEurope, 2012]

For background processes, such as energy generation, oil refining, or p-xylene production, the temporal reference can be stated with a time period from 2009 to 2011. Transport process data refers to the years 2000-2012.

Geographical Reference

Primary production data from 12 production lines at 10 production sites in Europe was provided, comprising sites in the following countries: Belgium, Germany, Lithuania (2 lines), the Netherlands, Poland, Spain (4), United Kingdom (2). As stated by CPME, further plants were operating in Germany (1), Portugal (1), Spain (1) and Italy (2), but did not participate in the present study. The participating plants covered 2.9×10^6 t/year nameplate capacity representing 85% of the total European nameplate capacity (3.4×10^6 t/year). PET imported to Europe is not considered in this Eco-profile.

Cut-off Rules

In this Eco-profile any cut-off of material and energy flows has generally been avoided. For the Sb catalyst and other intermediate materials (with total input < 1% of PET output), e.g. H_3PO_4 , generic datasets from the LCA database Ecoinvent 3.3 [Ecoinvent, 2016] were used.

Simplified generic processes were assumed for a few additives like toners with missing secondary production data (with total input < 0.1% of PET output). The input/output relation of these processes has been determined by reaction equations from literature. The upstream production of the applied chemicals are modelled using Ecoinvent 3.3 data. Thus, the potential environmental relevant metal extraction and refinement processes are included in the LCI data.

Waste for recycling is generally cut off in Ecoinvent datasets. Furthermore, expenses for capital equipment were not considered in this Eco-profile.

Data Quality Requirements

Data Sources

This Eco-profile and EPD uses average data representative of the respective foreground production process, both in terms of technology and market share. The primary data are derived from site-specific information for processes under operational control supplied by the participating member companies of CPME (see Producer Description).

Foreground Processes

Primary or foreground data comprises all information concerning processes under operational control of the respective producer. The data are collected from the participating member companies of CPME and their plants. Collection of primary data was arranged by using electronic questionnaires for the manufacturing process and a potential on-site energy supply. The questionnaires were used to collect information about 'inputs and outputs of all materials and energy', 'releases to air', 'releases to water (after water treatment)' and 'transport and waste' of the considered production processes. A schematic overview of requested data is given in Figure 4.

The selection of substances for air and water release is based on the PRTR list (Pollution Release and Transfer Register; [European Commission, 2006]) from the EU regulation and the POP protocol of UNECE (persistent organic pollutants). Therefore all substances should – in principle – be known for these reporting requirements (assuming that also the quantity is known for the PRTR substances not surpassing the reporting threshold). Some few specifically relevant substances had been added, which are typical for PET production (e.g. acetaldehyde, ethylene glycol). For every data point the data supplier was asked to define the type of 'data classification' as 'measured', 'calculated' or 'estimated'.

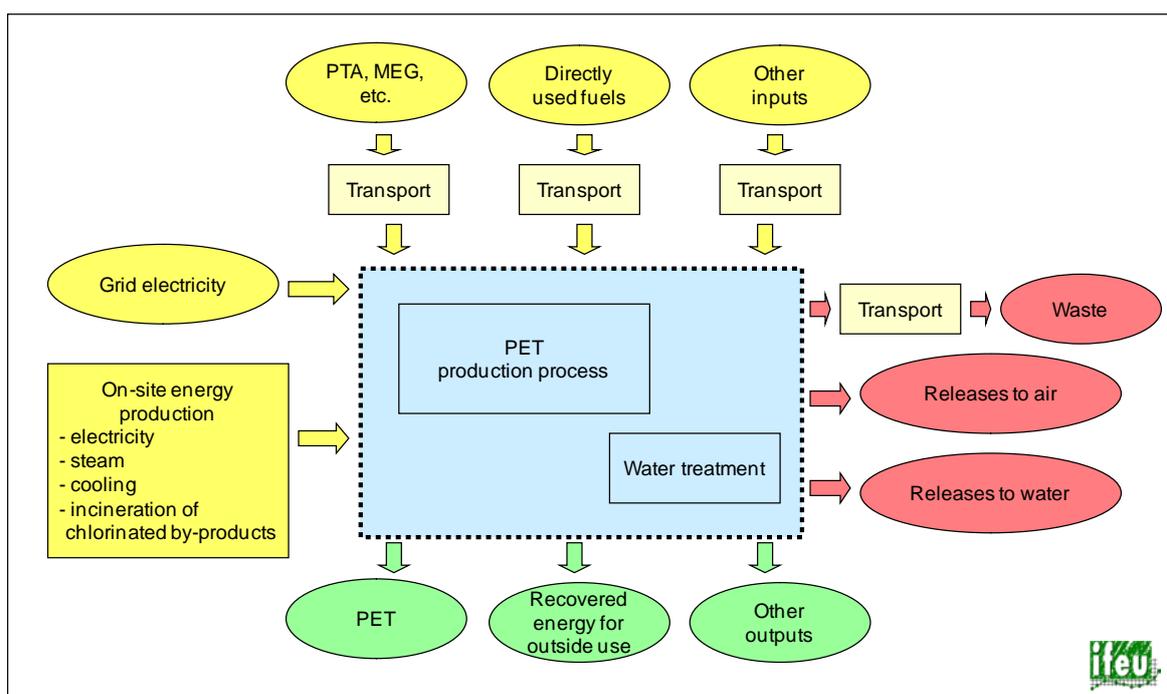


Figure 4: Schematic overview of considered material and energy flows of the sub-system PET production (the dotted line defines the system boundary).

Background Processes

Secondary or background processes are defined as processes that are either outside the operational control of the respective producer, or for which primary data are not available at a feasible effort. Generic datasets for these processes can be derived from literature, publicly available or commercial LCI databases. The most important background processes and its data sources are listed below.

PTA production

Data for PTA production was taken from the recently published EPD and Eco-profile of purified terephthalic acid (PTA) [CPME, 2016] of which the full dataset is known to the LCA practitioner. In this publication, the modelling for the PTA production process is based on primary data from five European PTA producers covering 79 % of the PTA production in Europe.

Production of ethylene glycol

The modelling of the steam cracking process and the subsequent conversion of ethylene to ethylene glycol was taken from the recently published EPD and Eco-profile of steam cracker products [PlasticsEurope, 2012], of which the full dataset is known to the LCA practitioner. In this publication, the modelling of the steam cracking processes was based on confidential data provided by plant operators as well as on representative literature data. Furthermore, the Association of Petrochemicals Producers in Europe (APPE) provided recent data for energy consumption, feedstock mix and CO₂ emissions for the majority of European plants.

Production of p-xylene

Data concerning p-xylene production was taken from the recently published EPD and Eco-profile of BTX aromatics [PlasticsEurope, 2013], of which the full dataset is known to the LCA practitioner. In this publication, the modelling of the processes for BTX aromatics extraction and production is based on representative literature data. Additionally, the Aromatics Producers Association (APA), a sector group of APPE, checked and verified the data basis, especially the shares of feedstock mix and specific process data.

Upstream chains of fuels

Natural gas is commonly used as fuels for the on-site production of power or heat, i.e. in the form of process steam. For the compilation of this Eco-profile, up-to-date data of the upstream chain of natural gas, which had been collected and implemented recently, could be used. These data are based on the database Ecoinvent v3.3 [Ecoinvent, 2016]. A regional provenance mix according to the respective production site was considered using statistical data from Eurostat for the year 2012. The upstream chain for natural gas was updated with primary data for the main production countries/regions, especially in terms of their inputs and outputs. These primary data derive from the environmental/annual reports either of associations of the oil and gas producing industry or directly from important producers representing specific regions (e.g. the North Sea region, Russia, OPEC countries). Furthermore, data from scientific studies were used for the update of the upstream chain of natural gas.

Electricity production

Electrical power supply was modelled using country specific grid electricity mixes, since the environmental burdens of power production vary strongly depending on the electricity generation technology. The country-specific electricity mixes were obtained from a master network for grid power modelling maintained and annually updated at IFEU as described in ifeu [2016]. This network considers the basic power plant types and their respective raw material processes. Applying network parameters, the fuel mix and essential technical characteristics of each energy system are freely adjustable. The national grid electricity mix for each European country has been calculated using this network. The choice of parameters

was based on national electricity mix data by Eurostat [2014] for the reference year 2012 for all countries.

The system boundaries of the electricity module include:

- Power plant processes for electricity generation using coal and lignite, fuel oil, natural gas, biomass and waste as well as nuclear, hydroelectric, geothermal, solar and wind power;
- Upstream fuel chains in the case of coal, lignite, fuel oil, natural gas, biomass and nuclear power;
- Distribution of electricity to the consumer with appropriate management and transformer losses.

The network also includes combined heat and power generation. The share of district heat produced in coupled form is adjustable according to the power plant type. An allocation of the burdens to electricity and district heat is performed through allocation based on exergetic values of products. Additional information concerning the applied electricity grid model can be found on the website of IFEU. For electricity input to the foreground processes, the electricity mix of the respective country was used, whereas for electricity input to background processes a European average was applied.

Transport

For transport processes the main data sources are

- Rail: EcoTransIT World [ifeu et al., 2014]
- Road: Handbook Emission Factors for Road Transport [INFRAS, 2014]
- Ship: EcoTransIT World [ifeu et al., 2014]
- Pipeline: Ecoinvent v3.3 [Ecoinvent, 2016]

On-site energy and utilities

Steam and electricity production on-site was modelled using a generic steam boiler or CHP unit based on secondary data from several IFEU projects and the Ecoinvent 3.3 database using the primary data from each production site for fuel mix and efficiencies.

Sources for other utilities are:

- Compressed air (low and high pressure): Several data from IFEU projects, Ecoinvent 3.3 and the BREF on energy efficiency [European Commission, 2009]
- Industrial gases: oxygen and nitrogen according to Ecoinvent and IFEU internal database
- Process water: Ecoinvent 3.3

For raw materials with low mass contribution LCI data from Ecoinvent 3.3 are used; the most relevant materials are listed below (relevance is defined in this context as material mass per total PET output):

- Phosphoric acid (<0.1 %)
- Sulphuric acid (<0.1 %)
- Antimony (<0.1 %)

Since the metal components of catalysts can have a high influence on the impact category Abiotic Depletion Potential of minerals and ores (ADP elements), the extraction of Antimony was taken into account based on the metal content provided by PET producers.

Relevance

With regard to the goal and scope of this Eco-profile, the collected primary data of foreground processes are of high relevance, i.e. data from the most important producers in Europe in order to generate a European industry average production. Background processes, particularly the PTA and MEG production

including their upstream chains of steam cracking, aromatics separation, oil refining and grid electricity are also of high relevance for the Eco-profile. The environmental contributions of each process to the overall LCI results are shown in Chapter 'Life Cycle Impact Assessment.

Representativeness

Primary and secondary data were collected or updated according to goal and scope of this PET Eco-profile.

Plants providing primary data were responsible for 2.9 Mt of installed PET production capacity in Europe in 2014. This reflects a coverage of about 85 % of the installed production capacity in Europe (3.4 Mt). The used data reflect the current technology in Europe and the current upstream chains of feedstock relevant for production in EU27 member countries.

Consistency

To ensure consistency only primary data of the same level of detail and background data from the databases were used. While building up the model, crosschecks concerning the plausibility of mass and energy flows were continuously conducted. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system.

Reliability

Data reliability ranges from measured to estimated data. Data of foreground processes provided directly by producers were predominantly measured. For emissions to air and to water the type of data source is varying from site to site with a tendency that standard emissions are measured – e.g. emissions to air as nitrogen oxides, sulphur dioxide, methane and emissions to water as biological and chemical oxygen demand, suspended solids, total nitrogen or phosphorous. Carbon dioxide emissions to air are mostly calculated by the amount of fuel used. Other emissions are measured, calculated, and also estimated at PET plants.

Data of relevant background processes, e.g. grid electricity, is based on IFEU models that are regularly updated with statistical data, with available primary data, and with data derived from literature after it has been reviewed and checked for its quality.

Completeness

In general the collected and applied data could be stated as complete, because no flows are omitted or substituted. However, not every detail process with its potential emissions at the individual plants is known. Depending on the site, very different numbers of parameters have been filled in the questionnaires of one and the same process step. This suggests that the amount of parameters measured could be also site dependent. Thus the data is considered as complete for all relevant flows.

Several emissions to air were considered to be mandatory for combustion processes (CO, CO₂, NO_x, CH₄) and PET production (ethylene glycol, acetaldehyde). In case, a production unit did not report a value for these substances, the weighted average value of the reporting units was used. The same approach was used for missing transport distances.

Precision and Accuracy

The relevant foreground data consist of primary data or modelled data based on primary information sources of the owner of the technology, such that the best possible precision has been achieved within

this goal and scope. The accuracy of results with respect to systematic errors can be considered very high due to the high level of detail within both, input data and model.

Reproducibility

All data and information used either are documented in this report or are available from the mathematical model of the processes and process plans designed within the Umberto 5.6 software. The reproducibility is given for internal use since the owners of the technology provided the data and the models are stored and available in a database. Sub-systems are modelled by 'state-of-art' technology using data from a publicly available and internationally used database. It is worth noting that for external audiences, it may be the case that full reproducibility in any degree of detail will not be available for confidentiality reasons. However, experienced experts would easily be able to recalculate and reproduce suitable parts of the system as well as key indicators.

Data Validation

The data on PTA production was collected from participating companies in an iterative process with several feedback steps if necessary. The collected data was validated using existing data from published sources or expert knowledge.

The relevant background information from those sources mentioned under 'data sources' has been validated and is regularly updated by the LCA practitioner.

Life Cycle Model and Calculation Rules

The life cycle system is modelled in Umberto 5.6, a standard software tool for LCA. The associated database integrates ISO 14040/44 [ISO, 2006a; b] requirements. Due to confidentiality reasons, details on software modelling and methods used cannot be shown here. Data for production processes have been transferred to the model after a successful data validation. Background data has been added from the IFEU LCI database and other sources as described in the Section "Data Sources". The calculation follows the vertical calculation methodology, i.e. that the averaging is done after modelling the specific processes.

Vertical Averaging

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages are calculated as far as possible (Figure 5). These vertical averages comprise the PET production unit itself, the on-site energy supply (electricity and steam if produced on-site), on-site production of supply materials like pressurised air, nitrogen, or process water, transport of input materials and waste, waste treatment, and wastewater treatment. National electricity mixes were used to calculate the grid electricity supply. For all other material input, including PTA and MEG, European average datasets were used, hence horizontal averaging was applied in these cases.

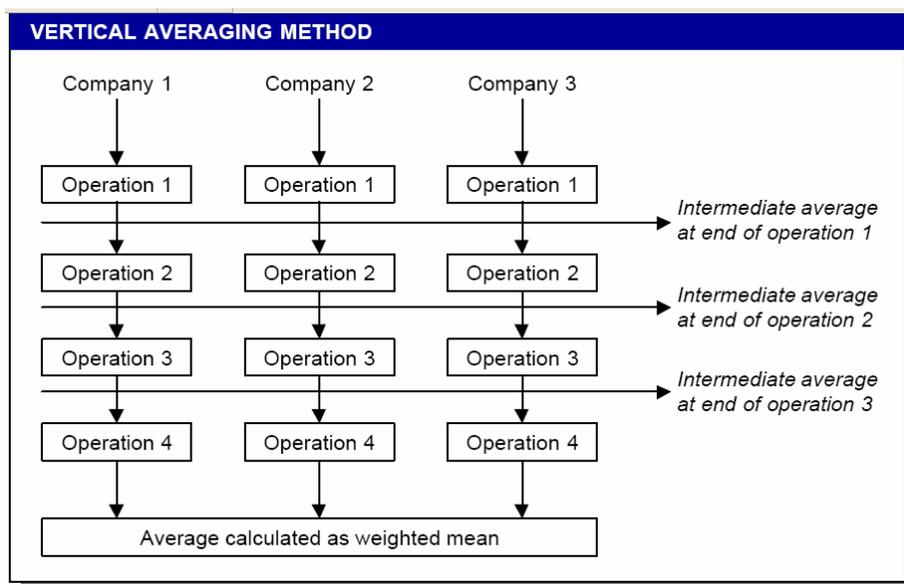


Figure 5: Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001).

Allocation Rules

Production processes in chemical and plastics industry are usually multi-functional systems, i.e. they have not one, but several valuable product and co-product outputs. According to PlasticsEurope methodology [PlasticsEurope, 2011a], allocation should be avoided by expanding the system to include the additional functions related to the co-products, wherever possible. System expansion should only be used where there is a dominant, identifiable displaced product, and if there is a dominant, identifiable production path for the displaced product.

Often, however, avoiding allocation is not feasible in technical reality, as alternative stand-alone processes do not exist in reality or alternative technologies show completely different technical performance and product quality output. In such cases, the aim of allocation is to find a suitable partitioning parameter so that the inputs and outputs of the system can be assigned to the specific product sub-system under consideration. In principle, allocation rules should reflect the goal of the production process.

In general, physical or economic allocation was applied in this study. The foreground process of PET manufacturing has no relevant by-products except for small amounts of amorphous PET (<1 wt.-% of total output) and 'off-spec PET' (about 0.1 wt.-% of total output). For these products the following allocation factors were applied:

- Amorphous PET: allocation factor of 0.67; this factor was derived by dividing the polymerisation process into two sub-processes for a) esterification and melt polymerisation and b) solid state polymerisation. Energy requirements for both processes have the following shares on total energy requirement: a) 67 % and b) 33 %.
- Off-spec PET: allocation factor of 0.3, based on relative price compared to bottle grade PET

For the background processes aromatics separation, steam cracking and oil refining the following allocation rules were used:

- Most of the unit processes in BTX aromatics extraction and production yield more than one product. In these cases, the feedstock input is allocated by mass to all products leaving the process (following the law of conservation of mass), whereas all the other inputs and outputs (energy + other input, emissions and solid wastes) are allocated by mass only to the Intended Products (IP) benzene, toluene, and xylenes.
- Steam cracking of liquid or gaseous feeds yields several products, which in part are internally used as fuel or feedstock. This internal recycling is modelled as closed-loop and does not lead to additional products of the considered sub-system. Diverse hydrocarbons are generated as co-products next to ethylene, propylene, hydrogen, butadiene and pyrolysis gas. The shares of the co-products can vary significantly depending on plant configuration, market values of products and feedstock composition – ethylene and propylene are the dominating products if naphtha is used as feedstock. The feedstock input is allocated by mass to all products leaving the cracking plant. All the other inputs and outputs, i.e. energy input, emissions and solid wastes, are allocated by mass to the Intended Products (IP), i.e. ethylene, propylene, butadiene, benzene, toluene, xylenes and purified hydrogen. APPE applied this allocation procedure in the European Emission Trading System (EU ETS) and recommends its application also in this study to keep consistency.
- An oil refinery is a complex production sub-system with many multi-output processes and products. The basic allocation criterion is the energy of products on a detailed process level. Since the majority of the products of the petroleum refinery are used for energy application the calorific value is the preferable coefficient. For this reason and as the EU Renewable Energy Directive recommends energy allocation for biofuels, bio-liquids and their fossil fuel comparators, refinery processes have been allocated by energy. The intention of every process has been considered defining the allocation keys between expenses and revenues, e.g. the catalytic cracking process (in refineries) is a conversion process to upgrade heavier hydrocarbons into more valuable lower boiling hydrocarbons. The feed stream, which is usually heavy vacuum distillate, is allocated to all product streams by energy. But other expenses, such as energy and catalysts input or emissions, are allocated by energy only to the desired lighter products; the cracker residue does not receive any energy or emission burdens besides the material feed demand.
- The emissions that crude oil extraction and natural gas processing cause within a specific supply region were basically allocated by mass. This is especially relevant for regions where a combined gas and oil production takes place.

The allocation rule for waste management is the following: process waste with a recycling potential (e.g. catalysts) leaving the system (<0.5 wt.-% of the total output) does not receive any burdens or credits (Cut-Off). Other process waste is treated within the system.

Life Cycle Inventory Results

The LCI results of bottle grade PET are not completely shown in this report due to its large size. They are available in separated documents on the website of PlasticsEurope (www.plasticseurope.org). For primary energy demand a detailed analysis is presented in chapter “Energy Demand”. Other key LCI indicators are shown in chapter “Other LCI Key Indicators”.

Formats of LCI Dataset

The Eco-profile for bottle grade PET is provided in three electronic formats:

- As input/output table in Excel[®]
- As XML document in EcoSpold format (www.ecoinvent.org)
- As XML document in ILCD format (<http://lct.jrc.ec.europa.eu>)

Key results are summarized in the following sections.

Energy Demand

As a key indicator on the inventory level, the **primary energy demand** (system input) shown in Table 1 indicates the cumulative energy requirements at the resource level, accrued along the entire process chain (system boundaries), quantified as gross calorific value (upper heating value, UHV). The net calorific value (lower heating value, LHV) is also presented in Table 1 for information purposes.

As a measure of the share of primary energy incorporated in the product, and hence indicating a recovery potential, the **energy content in the polymer** (system output), quantified as the gross calorific value (UHV) is shown in Table 1 as well.

Table 1: Primary energy demand (system boundary level) per 1 kg PET

Primary Energy Demand	Value [MJ]
Energy content in PET (energy recovery potential, quantified as gross calorific value of PET)	24.0
Process energy (quantified as difference between primary energy demand and energy content of PET)	47.2
Total primary energy demand (Upper heating value)	71.2
Total primary energy demand (lower heating value)	66.4

Using fossil fuels in combustion processes is related to many important environmental impacts. Hence, the primary energy demand is often a good proxy for the environmental performance of a life cycle of a product system.

Consequently, the difference (Δ) between primary energy input and energy content in PET output is a measure of **process energy** that may be either dissipated as waste heat or recovered for use within the system boundaries. Useful energy flows leaving the system boundaries were removed during allocation.

Table 2 shows how the total energy input (primary energy demand) is used as fuel or feedstock. Fuel use means generating process energy, whereas feedstock use means incorporating hydrocarbon resources into the polymer precursor. Note that some feedstock input may still be valorised as energy; furthermore, process energy requirements may also be affected by exothermic or endothermic reactions

of intermediate products. Hence, there is a difference between the feedstock energy input and the energy content of the polymer precursor (measurable as its gross calorific value).

Table 3 shows the distribution of the primary energy demand between renewable and non-renewable resources. Since the plants within the scope of this study are exclusively using raw materials produced from fossil resources (crude oil and natural gas), the share of non-renewable energy resources is close to 100 %. The small share of renewables is mainly caused by the national electricity mixes.

In Table 4 the types of useful energy inputs in the PET production (foreground process only!) are analysed: thermal energy plays a major role compared to electric energy.

Table 2: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg PET

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	1.66	0.081		1.66
Oil	47.07	1.028	32.41	14.66
Natural gas	16.74	0.362	1.73	15.01
Lignite	1.08	0.101		1.08
Nuclear	3.04	4.85E-06		3.04
Other non-renewable fuels	0.00			0.00
Biomass	0.89			0.89
Hydro	0.45			0.45
Solar	0.05			0.05
Geothermic	0.00			0.00
Wind	0.25			0.25
Other renewable fuels	0.00			0.00
Sub-total renewable	1.6	0.0	0.0	1.6
Sub-total Non-renewable	69.6	1.6	34.1	35.5
Total	71.2	1.6	34.1	37.1

Table 3: Primary energy demand by renewability per 1 kg PET

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	1.6	2.3%
Non-renewable energy resources	69.6	97.7%
Total	71.2	100.0%

Table 4: Analysis by type of useful energy for PET production process per 1 kg of PET

Type of useful energy in process input	Value [MJ]
Electricity	0.72
Imported steam (calculated as LHV of fuel, 90% efficiency)	0.43
Fuel directly fed to plant (as LHV of fuel)	2.28
Total (for selected key process)	3.43

Water Use and Consumption

Table 5 shows the water use (i.e. water input only) for the PET production process (foreground process only!) whereas Table 6 shows the water use along the total process chain from cradle to gate. Table 7 shows the water consumption (i.e. water output is subtracted from input when fed back to the same water body) for both PET production process and the whole production chain.

Table 5: Gross water resources used in foreground processes (PET production including on-site utilities) per 1 kg of PET

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	0.1	0.3	0.5
River/canal	0.1	2.0	2.1
Sea	0.0	0.0	0.0
Unspecified	0.0	7.1	7.1
Well	0.3	0.1	0.4
Totals	0.5	9.6	10.1

Table 6: Gross water resources used in the total process chain (cradle-to-gate) per 1 kg of PET

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	0.1	0.3	0.5
River/canal	0.8	24.9	25.8
Sea	0.8	4.5	5.3
Unspecified	4.3	58.7	63.0
Well	0.6	0.6	1.1
Totals	6.7	89.0	95.8

Table 7: Water consumption per 1 kg of PET

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Foreground processes only	0.5	0.9	1.4
Total process chain	6.7	42.1	48.8

Air Emission Data

Table 8 shows a few selected air emissions for the PET production process (foreground process only!) which are commonly reported and used as key performance indicators.

Table 8: Selected air emissions of the foreground processes (PET production including on-site utilities) per 1 kg of product

Air emissions	kg
Carbon dioxide, fossil [kg]	0.18
Carbon monoxide (CO) [kg]	2.63E-04
Sulphur dioxide (SO ₂) [kg]	3.34E-04
Nitrogen oxides (NO _x) [kg]	6.74E-04
Particulate matter ≤ 10 µm [kg]	5.98E-05
Non-methane volatile organic compounds (NMVOC) [kg]	5.31E-05
Ethylene glycole [kg]	3.29E-06
Acetic acid [kg]	2.08E-06

Wastewater Emissions

Table 9 shows a few selected wastewater emissions for the PET production process (foreground process only!) that are commonly reported and used as key performance indicators.

Table 9: Selected water emissions of the foreground processes (PET production including on-site utilities) per 1 kg of PET

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	1.80E-04
Chemical oxygen demand (COD)	6.53E-04
Total organic carbon (TOC)	2.40E-04
Chloride, ion	3.33E-04
Sodium, ion	3.07E-05
Sulphate	1.95E-05
Suspended solids	8.55E-04

Solid Waste

Table 10 shows the solid waste generated from the PET production process before treatment (foreground process only!) whereas Table 11 shows the solid waste generated along the total process chain from cradle to gate after waste treatment leaving the system.

Table 10: Solid waste generation of the PET production process (before treatment) by type and destination per 1 kg of PET

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	8.9E-05	1.6E-04	6.5E-04	9.5E-05	1.0E-03
Hazardous	5.8E-05	8.6E-04	2.8E-04	1.0E-05	1.2E-03
Unspecified	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Total	1.5E-04	1.0E-03	9.3E-04	1.1E-04	2.2E-03

Table 11: Solid waste generation of the total process chain (cradle-to-gate, after treatment) by type and destination per 1 kg of PET

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous			8.78E-03		8.78E-03
Hazardous			2.95E-04		2.95E-04
Unspecified			1.92E-06		1.92E-06
Total			9.08E-03		9.08E-03

Life Cycle Impact Assessment

Input

Natural Resources

The Abiotic Depletion Potential (ADP) measures the extraction of natural resources such as iron ore, scarce minerals, and fossil fuels such as crude oil. This indicator is based on ultimate reserves and extraction rates. It is distinguished into the two subcategories 'ADP, elements' and 'ADP, fossil fuels'. For 'ADP, elements' Antimony (Sb) is used as a reference for the depletion of minerals and metal ores and for 'ADP, fossil fuels' the lower heating value (LHV) of extracted fossil fuels is considered. It is calculated according to updated characterisation factors of CML [CML, 2015]. 'ADP, fossil fuels' is not identical with the 'Primary Energy Resource Input' since the latter is based on upper heating values and ADP is based on lower heating values. Furthermore, 'ADP, fossil fuels' includes neither renewable resources nor uranium.

Table 12: Abiotic Depletion Potential per 1 kg PET

Natural resources	Value
Abiotic Depletion Potential (ADP). elements [kg Sb eq]	2.41E-04
Abiotic Depletion Potential (ADP). fossil fuels [MJ]	62.0

Output

Climate Change

The impact category climate change is represented by the Global Warming Potential (GWP) with a time horizon of 100 years. The applied characterisation factors are based on the last report of the Intergovernmental Panel on Climate Change [IPCC, 2013].

Table 13: Global Warming Potential (100 years) per 1 kg PET

Climate change	kg CO ₂ eq.
Global Warming Potential (GWP)	2.19

Acidification

The Acidification Potential (AP) is quantified according to Hauschild / Wenzel [1998] with updated characterisation factors of CML [CML, 2015].

Table 14: Acidification Potential per 1 kg PET

Acidification of soils and water bodies	g SO ₂ eq.
Acidification Potential (AP)	6.47

Eutrophication

The Eutrophication Potential (EP) is calculated according to Heijungs et al. [1992] with updated characterisation factors of CML [CML, 2015].

Table 15: Eutrophication Potential per 1 kg PET

Eutrophication of soils and water bodies	g PO ₄ ³⁻ eq.
Eutrophication Potential (EP), terrestrial	0.52
Eutrophication Potential (EP), aquatic	0.97
Eutrophication Potential (EP), total	1.49

Ozone Depletion

The calculation of Ozone Depletion Potential (ODP) is based on characterisation factors of the World Meteorological Organisation [WMO, 2014]. This implies also the consideration of bromomethane (methyl bromide) as ozone depleting substance with an ODP of 0.66 kg CFC-11 eq. per kg of bromomethane. This emission plays a major role for the overall ODP result of PET (about 96 %). Bromomethane is an unwanted side product of the PTA production. It has to be noted that only two of five PTA production units reported emissions of bromomethane [CPME, 2016] even though this emission is inevitably occurring during PTA production. In CPME [2016] units that did not report these emissions were attributed the weighted average of the reporting units. Bromomethane emissions can be greatly reduced through either catalytic oxidation or regenerative thermal oxidation of the waste gases followed by scrubbing.

Table 16: Ozone Depletion Potential per 1 kg PET

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	0.0184

Summer Smog

The Photochemical Ozone Creation Potential (POCP) is quantified according to Derwent et al. [1998] and Jenkin / Hayman [1999] with updated characterisation factors of CML [CML, 2015]. Known single substances were considered with their specific characterisation factor. For the calculation of POCP the group species "non-methane volatile organic compounds" (NMVOC) was also taken into account under the assumption of a conservative impact factor of 1.0 kg Ethene eq./kg NMVOC¹. Thus, the contribution of NMVOC to POCP is 78 % (1.80 g Ethene eq./kg PET).

¹ The characterisation factor for NMVOC proposed by CML is 0.15, which is considered too low for this case. However, a solid calculation of the characterisation factor is not possible as the exact composition is not known and an estimation is connected with high uncertainties. The applied factor of 1.0 is very conservative but in combination with the given amount of NMVOC can be seen as a simple basis for applying other characterisation factors.

Table 17: Photochemical Ozone Creation Potential per 1 kg of PET

Photochemical ozone creation potential	g Ethene eq.
POCP from NMVOC	1.80
POCP from other substances	0.51
POCP, total	2.31

Dust & Particulate Matter

Particulate matter with an aerodynamic diameter of less than 10 µm (PM10) is suspected to cause heart and circulatory diseases. Studies from internationally recognised organisations (e.g. WHO [2006]) confirm a high mortality risk from fine dust.

Large scale air pollution of PM10 is caused by direct emissions of particulate matter and secondary particles that are formed by precursors such as nitrogen dioxide (NO₂), sulphur dioxide (SO₂), ammonia (NH₃) and Non-Methane Volatile Organic Compounds (NMVOC). The characterisation factors shown in Table 18 are based on works of Heldstab et al. [2003] and De Leeuw [2002] for NMVOC.

Table 18: PM10 characterisation factors of air emissions according to Heldstab et al. [2003] and De Leeuw [2002].

PM10 and precursors	kg PM10 eq. / kg air emission
Particulate matter PM10	1.00
Secondary aerosol formers (precursors)	
NO _x (as NO ₂)	0.88
SO ₂	0.54
NH ₃	0.64
NMVOC	0.012

Table 19: Particulate matter emissions per 1 kg PET

Particulate matter		
Particulate matter ≤ 10 µm (direct emissions)	0.37	g PM10 eq.
Particulate matter ≤ 10 µm, secondary	5.27	g PM10 eq.
Particulate matter ≤ 10 µm, total	5.64	g PM10 eq.
Total particulate matter	5.94	g

Dominance Analysis

Table 20 shows the main contributions to the results presented above. In this context, foreground process refers to the PET production itself (including monomer purification, polymerisation reactors, extrusion, pelletising, heat exchangers, and compressors), thermal energy production, and on-site utilities like water preparation, wastewater treatment, and on-site generation of compressed air and nitrogen. Electric energy generation both on-site and in external power plants is considered in the category "electricity". "Waste treatment" includes the treatment of solid wastes from the PET production process and the transport of wastes to the respective treatment facility. The section "PTA production" refers to all processes connected to PTA production including thermal and electric energy supply and production of all raw materials except for p-xylene. The category "p-xylene production" includes all processes related to p-xylene production including all upstream processes, while "MEG refers to the same category of processes related to monoethylene glycol production from the extraction of fossil resources to factory gate. Other raw materials include the production of the antimony catalysts, phosphoric and sulphuric acid, and additives and their pre-chain. Transport includes the transport of all the materials directly fed to the foreground process (i.e. monomers, fuels, and raw materials).

It is shown in Table 20, that the production of p-xylene, PTA and MEG together is outstandingly dominating most of the impact categories with the highest contribution coming from p-xylene production. For 'Total Primary Energy', 'ADP, fossil', GWP, AP, ODP, POCP, PM10, and Water use, more than 80 % of the impact is created by p-xylene, PTA and MEG production and the related upstream chains. This is caused by the fact that the processes highly contributing to air emissions and to resource extraction are oil and gas extraction, transport, and refining, steam cracking of naphtha and other hydrocarbons, and p-xylene extraction. The detailed impact assessment of the upstream processes can be found in the respective Eco-profiles [CPME, 2016; PlasticsEurope, 2012, 2013]. It has to be highlighted that methylbromide (MeBr, also called bromomethane or Halon 1001) emissions from the PTA production process are responsible for more than 95 % of the ODP.

Nevertheless, foreground processes, especially for the generation of electrical and thermal energy contribute significantly (5-15%) to most of the impact categories. Of course, energy demand of the PET process requires combustion of fossil fuels leading to emissions of CO₂ (GWP), SO₂ and NO_x (AP and PM10) and depletion of fossil resources (ADP fossil). Contributions of the foreground processes to EP are mostly caused by NO_x emissions from combustion and from emission of nitrogen compounds to water. POCP relevant emissions are mostly NMVOC as a substance group but also acetaldehyde as process emission and combustion emissions carbon monoxide and sulphur dioxide. Water use on the foreground level is caused by cooling water input to both the process and to thermal energy supply. Treatment of solid wastes from the foreground processes has no significant contribution to the investigated impact categories.

Production of "other raw materials" to be used in the PET production significantly contributes to ADP elements and to EP. Both effects are by more than 98 % caused by extraction and refining of antimony being used as a catalyst.

Transport of input materials and fuels contributes to AP and PM10 (about 11 %). This is caused by SO₂ and NO_x emissions from combustion processes in ship engines. On average, input materials are transported more than 2400 km by ship.

Table 20: Dominance analysis of impacts per 1 kg PET

	Total Primary Energy	ADP Ele- ments	ADP Fossil	GWP	AP	EP	ODP	POCP	PM10	Water use
	MJ	kg Sb eq.	MJ	kg CO ₂ eq.	g SO ₂ eq.	g PO ₄ ³⁻ eq.	g CFC-11 eq.	g C ₂ H ₄ eq.	g PM10 eq.	kg
PET production (incl. thermal energy and utilities)	5.4%	0.0%	5.0%	8.0%	2.8%	2.6%	0.3%	3.6%	3.1%	0.0%
Electricity ^{a)}	2.6%	0.0%	1.9%	5.2%	4.0%	1.9%	0.3%	0.7%	4.0%	5.8%
Waste treatment ^{a)}	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Subtotal Foreground Processes	8.0%	0.0%	6.9%	13.2%	6.8%	4.5%	0.6%	4.4%	7.0%	5.8%
PTA production (excluding p-xylene)	13.6%	0.1%	11.9%	24.4%	14.9%	16.3%	96.6%	24.3%	15.4%	60.6%
p-xylene production	54.0%	0.0%	57.5%	36.0%	50.1%	43.6%	1.8%	45.5%	48.0%	15.3%
MEG production	23.9%	0.0%	23.1%	25.1%	16.3%	16.3%	0.9%	23.6%	16.9%	17.9%
Other raw materials	0.1%	99.9%	0.1%	0.2%	1.0%	14.1%	0.0%	0.3%	1.0%	0.3%
Transport of monomers and other raw materials	0.5%	0.0%	0.6%	1.1%	10.9%	5.1%	0.0%	1.9%	11.6%	0.1%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

^{a)} only relating to direct input/output of the PET production process

Comparison with previous Eco-profile

In general, a comparison of the current Eco-profile with the results of the previous study from 2011 [PlasticsEurope, 2011b] is not possible since all processes in the upstream chain have been updated within the last years. Additionally, in the 2011 Eco-profile the whole process chain was modelled at once without publishing each step separately. Furthermore, environmental impact characterisation factors are also subjected to continuous update causing changes in results of studies conducted in different time.

In Figure 6 the contribution analysis for the Global Warming Potential of the PET Eco-profile from 2011 is compared to the current results. As the feedstock input for PET production did only change marginally between the two studies it becomes clear that the changes in the Eco-profiles of upstream processes (PTA, p-xylene and MEG production) have a high impact on the results for PET. Overall, the GWP of PET did not change significantly between both studies since the uncertainty range can be estimated to be at least 10%.

Taking into account the (confidential) dataset of foreground systems which was compiled for the 2011 study (on the basis of 2008 production data) and the dataset collected for the current study (basis year 2015 production data), we can derive that the **thermal and electric energy requirements on the PET process level have decreased in this time period by about 10 % and by 30 %, respectively.** This

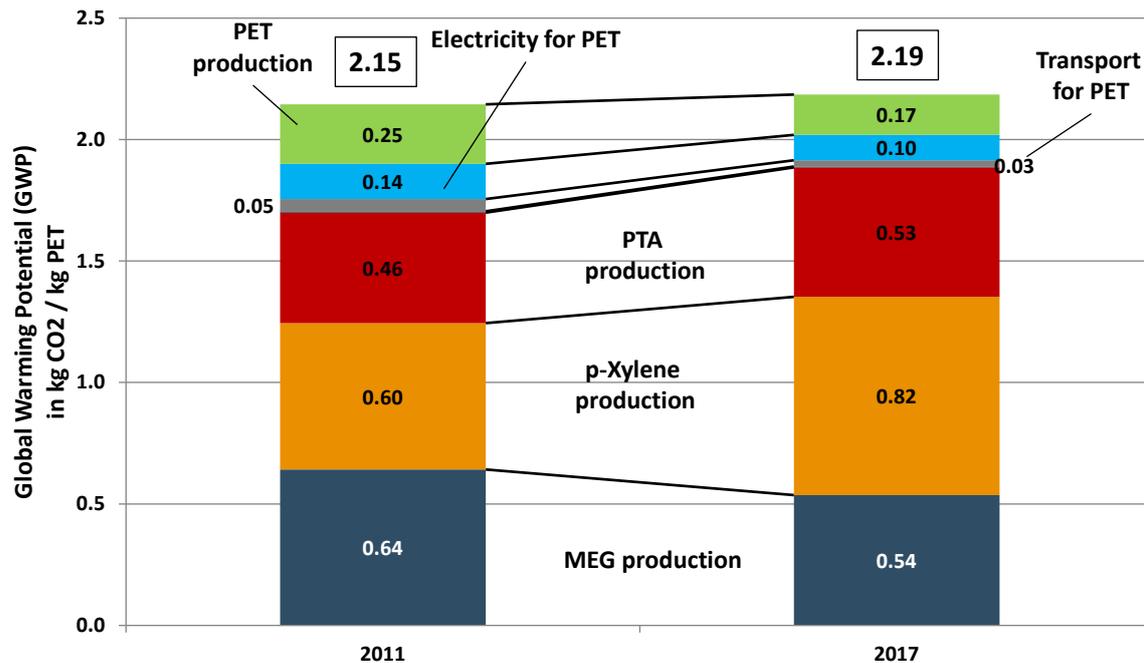


Figure 6: Contribution analysis for Global Warming Potential: Results of the 2011 Eco-profile and the current study in direct comparison.

leads to a reduction of the GWP directly caused by the PET production from 0.39 to 0.27 kg CO₂/kg PET (see also Figure 6).

To compare the system modelled in 2011 and the present production system a comparison scenario was developed which removes the differences that originate from the different background system models and environmental impact characterisation factors of materials. The following section describes this procedure in detail.

Comparison scenario: Same upstream processes for the 2011 & 2016 studies

As was shown before, the upstream processes of PTA and MEG production and their respective upstream chains are of high importance for the overall results of the Eco-profile of PET (see “Dominance Analysis” section). To eliminate differences caused by different assumptions and different data sets used in the current Eco-profile and in the previous version [PlasticsEurope, 2011b], a comparison scenario for the year 2008 was designed with the following features:

- original datasets for PTA and PET production referring to the year 2008, based on primary data (last data collection relating to the year of 2008)
- electricity grid mix for PTA and PET production for 2012 (as was used for the current study)
- using the same datasets for the upstream processes of p-xylene and MEG production (oil and gas extraction, refinery, steam cracker, aromatics extraction) that were used in the current study (referring to 2012 for p-xylene and 2011 for MEG)

Thus, the only difference between the model of PET production in 2015 and the adapted model of PET production in 2008 is in the production data for PTA and PET. All other upstream processes are equalised.

Table 21 shows the results of this comparison scenario for the year 2008 together with the current Eco-profile results and in Figure 7 the contribution analysis for GWP is shown for both calculations.

Despite the improvements on the foreground level, especially energy reductions within the PET production plants only very small reductions of the overall environmental impacts (especially for GWP and Primary Energy Demand) were realised. Having the dominance analysis in mind it becomes clear that the upstream processes crude oil extraction and refining, steam cracking, aromatics extraction and ethylene glycol production have very high environmental impacts leaving very little space for improvements at the end of the supply chain. However, realised reductions in Acidification Potential, Ozone Depletion Potential and Photochemical Ozone Creation Potential can directly be attributed to improvements in PTA and PET production:

- reduced emissions of SO₂ and NO_x led to a reduction in AP
- reduced emissions of methylbromide in PTA production led to reduction in ODP
- reduced emissions of NMVOC and NO_x led to a reduction in POCP

Notable is the increase of renewable energy use which is caused by one installation using biomass for steam generation. Biomass-based firing also partly contributed to the decreased GWP by its lower greenhouse gas emission compared to fossil fuel using technologies.

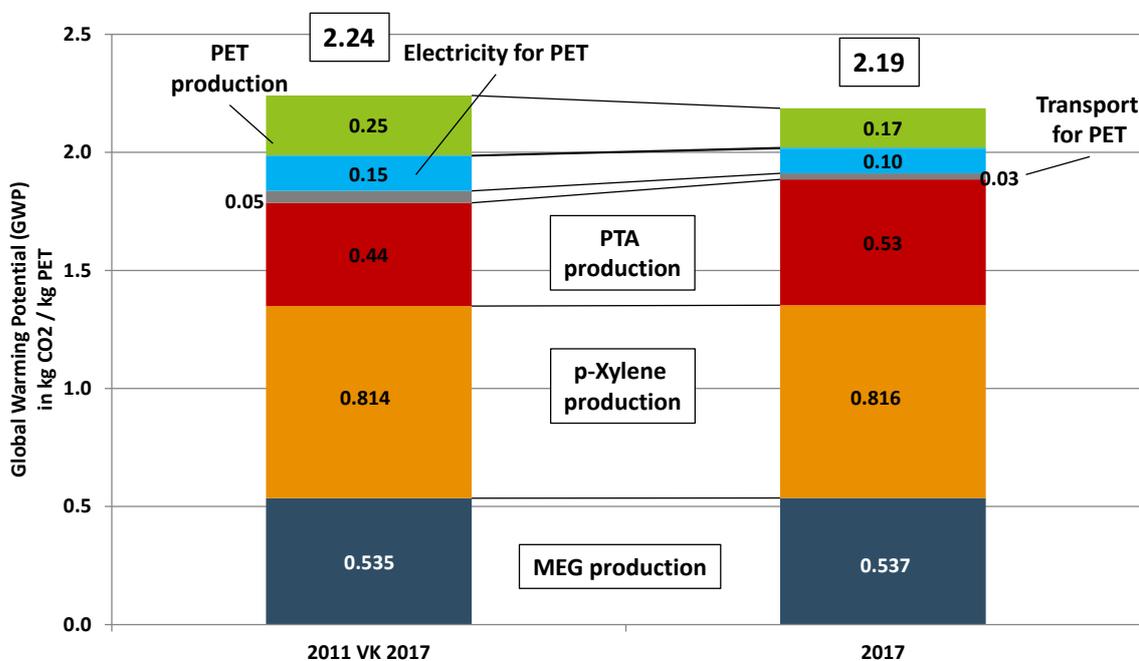


Figure 7: Contribution analysis for Global Warming Potential using the comparison scenario for the 2011 results (2011 VK 2017, see text for details) and the current study in direct comparison.

Table 21: Comparison of the present Eco-profile data of PET with the comparison scenario for 2008
(changes only in the foreground level of PTA and PET production)

Environmental Impact Categories	Eco-profile PET (2011) comparison scenario	Eco-profile PET (2016)	Difference
Gross primary energy from non-renewable resources [MJ]	69.70	69.60	-0.1%
Gross primary energy from renewable resources [MJ]	1.16	1.64	41.7%
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	2.52E-04	2.41E-04	-4.3%
Global Warming Potential (GWP) [kg CO ₂ eq.]	2.24	2.19	-2.5%
Acidification Potential (AP) [g SO ₂ eq.]	7.51	6.47	-13.9%
Eutrophication Potential (EP) [g PO ₄ ³⁻ eq.]	1.48	1.49	0.9%
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	0.0193	0.0184	-4.8%
Photochemical Ozone Creation Potential [g Ethene eq.]	4.34	2.31	-46.9%

External Independent Review Summary

The subject of this critical review is the development of the Eco-profile for bottle grade polyethylene terephthalate (PET).

The review process included revisions of the final Eco-profile report and various web-conferences between the LCA practitioner and the reviewer, which encompassed spot checks of data and calculations as well as comparisons with previous Eco-profiles of PET and its main precursors. Furthermore, the Eco-profile report was reviewed by industry participants and the representative of CPME. All questions and recommendations were taken forward to the LCA practitioner, and the report was adapted and revised accordingly.

Primary industry data were collected for the foreground processes comprising PET production and taking into account the specific production processes of the participating companies. Background data representing the main precursors, i.e. purified terephthalic acid (PTA) and mono ethylene glycol (MEG) were taken from existing Eco-profiles [CPME 2016; PlasticsEurope 2012]. All other relevant material and energy inputs were taken from the library of the dataset developer, representative literature data and the database Ecoinvent v3.3 (for details see p. 14ff. of the report). Primary industry data was collected from 7 European PET producers for 12 production plants, which lead to an estimated overall representativeness of 85% of the installed EU27 production capacity in 2015.

The potential environmental impacts for bottle grade PET are largely dominated by the precursors across all impact categories (except ADPe). The extraction and refining of antimony being used as a catalyst contributes with 98% to the impact category ADPe. The foreground processes related to PET production, in particular the generation of electrical and thermal energy, contribute significantly (5-15%) to most of the impact categories.

The direct comparison of results of this Eco-profile with a previous version published in 2011 is difficult due to differences caused by different assumptions and different data sets used in this and the previous version [PlasticsEurope 2011b]. Hence, a comparison scenario for the year 2008 was designed. This comparison shows small to substantial improvements with regards to the potential environmental burdens for PET production (see Table 21 in report).

The LCA practitioners have demonstrated very good competence and experience, with a track record of LCA projects in the chemical and plastics industry. The critical review confirms that this Eco-profile adheres to the rules set forth in the PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology and PCR for Uncompounded Polymer Resins and Reactive Polymer Precursors (PCR version 2.0, April 2011). As a result, this dataset is assessed to be a reliable and high quality representation of bottle grade PET produced in Europe.

Name and affiliation of reviewer:

Reviewer: Matthias Schulz, Schulz Sustainability Consulting on behalf of DEKRA Assurance Services GmbH, Stuttgart, Germany

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