



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

Purified Terephthalic Acid (PTA)

CPME

February 2016



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 2011]. EPDs provide environmental performance data, but no information on the economic and social aspects which 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 purified terephthalic acid (PTA) from cradle to gate (from crude oil extraction to PTA powder 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 performance of different materials and the effects of relevant life cycle parameters. 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	DEKRA Consulting GmbH
Number of plants included in data collection	5
Representativeness	Good (79 % of installed production capacity covered)
Reference year	2011-2013
Year of data collection and calculation	2013 and 2014
Expected temporal validity	2017
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 PTA in Europe from cradle to gate.

Production Process

Crude terephthalic acid (CTA) is produced by oxidation of p-xylene. A subsequent purification step leads to purified terephthalic acid (PTA).

In addition to these foreground processes, the following processes in the supply chain are considered for this EPD: 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).

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

Data Sources and Allocation

Confidential input and output data for the PTA production processes including on-site energy production was provided by five European PTA producers (primary data).

Data concerning the upstream processes p-xylene production, steam cracking, catalytic reforming, fossil fuels extraction and refinery were taken from the Eco-profiles of BTX aromatics [PlasticsEurope 2013] 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 PTA 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 v2.2 has been used to fill gaps where no primary data was available and to cross-check primary data.

Allocation within the foreground system was not necessary since it is a single output process. Concerning the background processes, allocation was intended to be avoided; where necessary, processes have been allocated by physical properties, such as mass, exergy, 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 this cradle-to-gate system: the object of this study is PTA, a raw material for PET production (poly ethylene terephthalate), 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 PTA.

Input Parameters

Indicator	Unit	Value
Non-renewable energy resources ¹⁾	MJ	55.1
• Fuel energy	MJ	23.7
• Feedstock energy	MJ	31.4
Renewable energy resources (biomass) ¹⁾	MJ	0.6
• Fuel energy	MJ	0.6
• Feedstock energy	MJ	0.0
Abiotic Depletion Potential		
• Elements	kg Sb eq	2.24E-07
• Fossil fuels	MJ	49.7
Water use	kg	72.1
• for process	kg	3.6
• for cooling	kg	68.6

¹⁾ Calculated as upper heating value (UHV)

Output Parameters

Indicator	Unit	Value
Global Warming Potential (GWP)	kg CO ₂ eq	1.56
Ozone Depletion Potential (ODP)	g CFC-11 eq	0.02
Acidification Potential (AP)	g SO ₂ eq	4.87
Photochemical Ozone Creation Potential (POCP)	g Ethene eq	1.87 ³⁾
Eutrophication Potential (EP)	g PO ₄ eq	1.03
Dust/particulate matter ($\leq 10 \mu\text{m}$) ²⁾	g PM10	4.09
Total particulate matter ²⁾	g	4.33
Waste	g	6.0
• Non-hazardous	g	1.7
• Hazardous	g	0.2
• Unspecified	g	4.0

²⁾ Including secondary PM10

³⁾ Including NMVOC (1.48 g Ethene eq./kg PTA)

Additional Environmental and Health Information

CPME has continued to fully support initiatives to improve the safety and environmental performance of PTA production. Changes in production methods have lead to near zero human exposure to process chemicals. The environmental treatment of process effluents is being continuously upgraded and now represents the best available technology. This is reflected in the reductions observed in the LCA parameters between the last and this LCA study.

Additional Technical Information

(Pure) Terephthalic Acid (PTA) production technology is constantly improving. New production processes and catalyst recovery methods lead to better quality products produced in a more efficient manner. High quality PTA produced today is key to the production of improved grades of Poly-Ethyleneterephthalate (PET). Using this high quality PTA, European PET products meet all of the very stringent existing and upcoming regulatory requirements particularly for food contact applications such as drinks bottles.

Additional Economic Information

Continual product and process innovation of (Pure) Terephthalic Acid (PTA) has led to energy savings in production, transportation and use of resources. PTA is a globally traded commodity and PTA European production facilities provide essential support to local and European economy. PTA production in Europe supports 100% of the European PET production which in turn fulfils around 80% of European demand.

Information

Data Owner

Committee of PET Manufacturers in Europe (CPME aisbl)

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Programme Manager & Reviewer DEKRA Consulting GmbH

This Environmental Product Declaration has been reviewed by DEKRA Consulting GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006. Registration number: PlasticsEurope 2014-004, validation expires on 31 December 2017 (date of next revalidation review).

Programme Owner

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For copies of this EPD, 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.
- PlasticsEurope 2013: Eco profiles and Environmental Product Declarations of the European Plastics Manufacturers - Benzene, Toluene, and Xylenes (Aromatics, BTX). PlasticsEurope, February 2013.



Goal & Scope

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 parts of the 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«, however, its reference flows are disparate, namely referring to a broad variety of polymers and precursors. This implies that, in accordance with ISO 14040–44, a direct comparison of Eco-profiles is impossible. While 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. The same goes for 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

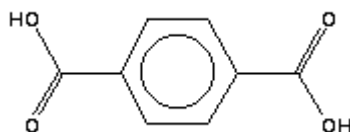
The Functional Unit and Declared Unit of this Eco-profile and EPD is:

1 kg of purified terephthalic acid (PTA) »at gate« (production site output), representing a European industry production average.

Product and Producer Description

Product Description

Terephthalic acid (CAS-Nr. 100-21-0) is a colourless to white crystalline organic compound, solid at room temperature (sublimes at 402 °C), and almost insoluble in water and alcohols. The molecular structure of terephthalic acid is shown below. Its gross calorific value is 19.2 MJ/kg [NIST 2011].



Terephthalic acid is mainly used for the production of polyethylene terephthalate (PET). For this process, a special grade is needed, called purified terephthalic acid (PTA), which contains over 99.99 wt.-% terephthalic acid and less than 25 ppm 4-carboxybenzaldehyde (4-CBA). Note that this Eco-profile uniquely deals with purified terephthalic acid.

The Commercial Production of PTA

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. Since the combination of bromine and acetic acid is highly corrosive, titanium or hastelloy lined equipment has to be used. 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). Temperature control is achieved by boiling point evaporation of acetic acid. Oxidation of p-xylene proceeds via several steps producing terephthalic acid with yields of more than 95 % at conversion of p-xylene of more than 98 %. 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 degassing 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.

Upstream Processes

Production of p-Xylene

The main source of xylenes in Europe (and the USA) is reformat (86 % in 2012) [APPE 2012], 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 nonaromatics (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. Toluene can also be fed to a hydrodealkylation (HDA) unit to produce additional benzene and methane. This is done either thermally at 550-800 °C and 30-100 bar or catalytically at 500-650 °C and 30-50 bar on alumina supported catalysts. Usually, hydrogen from refinery production is used for HDA.

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 charged 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.

Upstream Chains of Crude Oil and Natural Gas

Using up-to-date data of the steam cracker's upstream chains was a key issue for the compilation of this Eco-profile. To achieve this aim, the upstream chains of crude oil and natural gas from the Ecoinvent database v2.2 [ECOINVENT 2010] 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.

Upstream Processes Oil Refinery and Steam Cracking

The atmospheric distillation of crude oil within the refinery is of high relevance for the sub-sequent steam cracking. Most other energy and emission intensive processes of a refinery are more relevant for products that are usually not used as a steam cracker feedstock. Furthermore, the process of catalytic reforming of naphtha is of relevance, since reformat gasoline, one of its products, is used as a feedstock to the aromatic extraction and production plant.

For more detailed information on the processes of oil refining and steam cracking and the mathematical modelling please refer to PLASTICSEUROPE 2012, and PLASTICSEUROPE 2013.

Producer Description

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

- ARTLANT PTA SA, Portugal
- BP Aromatics Limited NV, Belgium
- CEPESA QUIMICA S.A., Spain
- Indorama Polymers Rotterdam B.V., The Netherlands
- Lotte Chemical UK Ltd, United Kingdom

Eco-profile – Life Cycle Inventory

System Boundaries

General Considerations

The Eco-profile refers to the **production of purified terephthalic acid** and is based on a **cradle-to-gate system** (Figure 1). 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 polymer production, conversion, use phase and end-of-life management are not included.

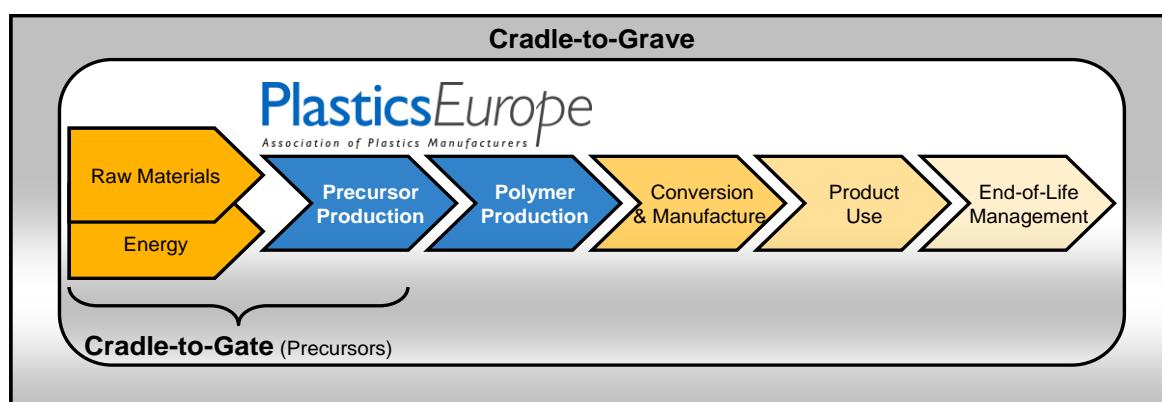


Figure 1: Cradle-to-gate system boundaries

Cradle-to-Gate System Boundaries for Production

The following processes are included in the cradle-to-gate LCI system boundaries (see also Figure 2):

- 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 production waste streams and related emissions generated by processes within the system boundaries

According to the methodology of Eco-profiles [PLASTICSEUROPE 2011] capital goods, i.e. the construction of plant and equipment as well as the maintenance of plants, vehicles and machinery are 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. An exception is low-radioactive waste from electricity generation for which a final storage has not been found yet; it is declared as output.

Technological Reference

The LCI data in this Eco-profile represent the average applied technology for the production of PTA in Europe as shown in Figure 2. They are based on confidential data collected from PTA 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. PTA imported to Europe is not considered in this Eco-profile.

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 years 2011 (2 plants), 2012 (2 plants), and 2013 (1 plant). Thus, the reference years for this Eco-profile are 2011-2013 with a maximum temporal validity until 2017. A new PTA production site started operating in 2011, while another site was closed in 2013. 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 2011].

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 2000-2009.

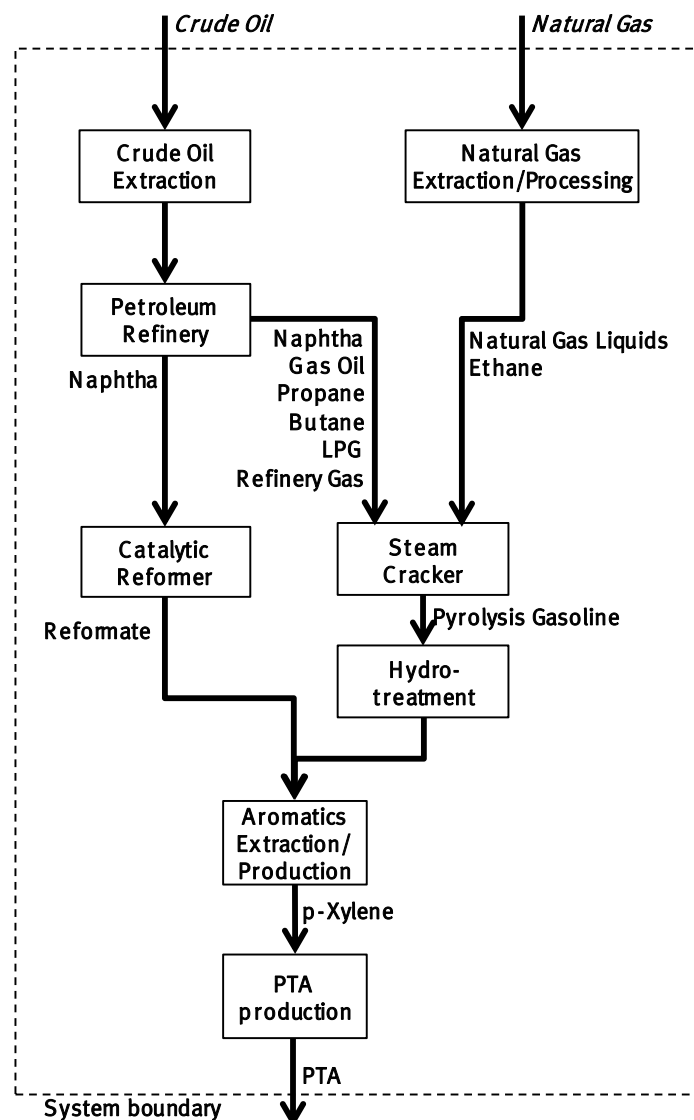


Figure 2: Schematic flow chart of the production processes for the polymer precursors under consideration (here PTA).

Geographical Reference

Primary production data from five PTA production sites in Europe were provided, comprising one site from each of the following countries: Belgium, the Netherlands, Spain, Portugal, and United Kingdom. As stated by CPME, further plants were operating in Germany (1), Poland (1), and Italy (1), but did not participate in the present study. The participating plants covered 3.2×10^6 t/year nameplate capacity representing 79 % of the total European nameplate capacity (4.1×10^6 t/year). PTA 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 acetic acid (input < 6 % of PTA output) and other commodities (with total input < 2% of PTA output), e.g. NaOH and HCl, generic datasets from the LCA database ecoinvent 2.2 [ECOINVENT 2010] were used.

Simplified generic processes were assumed for catalysts and a few commodities with missing secondary production data (with total input < 0.4% of PTA output). The input/output relation of the process has been determined by reaction equations from literature. The upstream production of the used metals (cobalt and manganese) and chemicals were implemented using ecoinvent 2.2 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 comprise all data concerning processes under operational control of the respective producer. The data were collected from the participating member companies of CPME and their PTA 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 sent to all participating companies. 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 3.

The selection of substances for air and water release was based on the PRTR list (Pollution Release and Transfer Register; PRTR 2006) from the EU regulation and the POP protocol of UN-ECE (Persistent Organic Pollutants). Therefore all substances should – in principle – be known for these reporting requirements (assuming that the quantities for the PRTR substances not surpassing the reporting threshold must be known in order to specify them as negligible). Some few specifically relevant substances have been added that are typical for PTA production (e.g. acetic acid, methyl acetate). For every data point the data

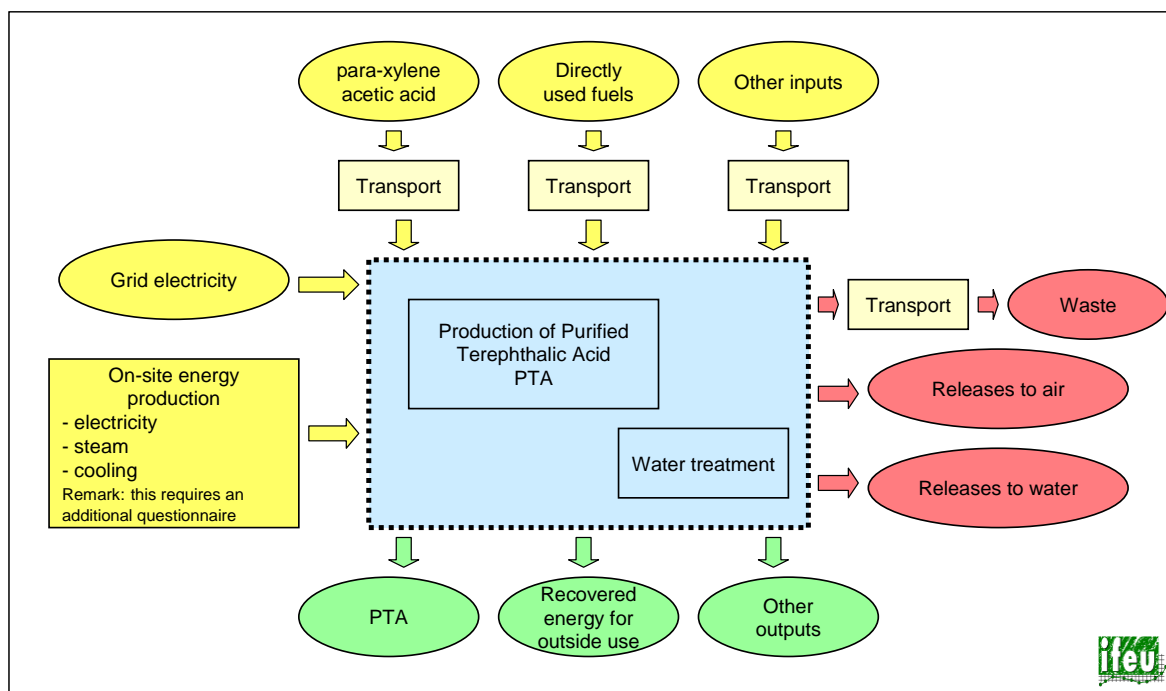


Figure 3: Schematic overview of considered material and energy flows of the PTA production (the dotted line defines the system boundary of the data collection)

supplier was asked to define the type of 'data classification' as 'measured', 'calculated' or 'estimated'.

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.

Data concerning p-xylene production was taken from the recently published EPD and Eco-profile of BTX aromatics [PLASTICEUROPE 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, such as data from the following databases and publications:

- Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry [BREF 2003]
- Ullmann's Encyclopedia of Industrial Chemistry [ULLMANN 2010]
- R. A. Meyers: Handbook of Petroleum Refining Processes [Meyers 2003]
- Methodology for the free allocation of emission allowances in the EU ETS post 2012 - Sector report for the chemical industry [ETS 2009]
- H.-G. Franck, J. W. Stadelhofer: Industrielle Aromatenchemie. Rohstoffe, Verfahren, Produkte [FRANCK 1987]
- S. Raseev: Thermal and Catalytic Processes in Petroleum Refining [RASEEV 2003]
- J.-P. Wauquier: Petroleum Refining 2. Separation Processes [WAUQUIER 2000]

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.

The modelling of the petroleum refinery was based on confidential process and emission data from several sites as well as on representative literature data from the following publications:

- Draft Reference Document on Best Available Techniques for Mineral Oil and Gas Refineries [BREF 2012]
- R. A. Meyers: Handbook of Petroleum Refining Processes [MEYERS 2003]

Statistical data for product mix and energy demand have been taken from the Eurostat database for the year 2011 [EUROSTAT 2013].

The modelling of the steam cracking processes 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 such as data from the following databases and publications:

- Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry [BREF 2003]
- Life cycle inventory database ecoinvent v2.2 [ECOINVENT 2010]
- Ullmann's Encyclopedia of Industrial Chemistry [ULLMANN 2010]

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.

Fuel oil and natural gas are commonly used as fuels for the on-site production of power or heat, i.e. in the form of process steam. Thus, it was necessary to represent their upstream chains adequately within this study to achieve appropriate LCI results, particularly with respect to air emissions. For the compilation of this Eco-profile, up-to-date data of the upstream chains of fuel oil and natural gas, which had been collected and implemented recently, could be used. These data are based on the database ecoinvent v2.2 [ECOINVENT 2010]. A regional provenance mix according to the respective production site was considered using statistical data from Eurostat for the year 2011. The upstream chains for crude oil and natural gas were 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.

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 2011. 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 [2013] for the reference year 2011 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.

For transport processes the main data sources are

- Rail: TREMOD (2009) and EcoTransIT (2008)
- Road HBEFA 2.1 and TREMOD (2009)
- Ship: Borken 1999 and ecoinvent v2.2 [Ecoinvent 2010]
- Pipeline: ecoinvent v2.2 [Ecoinvent 2010]

For production of on-site energy and utilities, the following sources were used:

- Steam and electricity:
Primary data from separate on-site energy questionnaire and secondary data from several IFEU projects and ecoinvent v2.2 [Ecoinvent 2010]
- Compressed air (low and high pressure):
Several data from IFEU projects, ecoinvent v2.2 [Ecoinvent 2010] and BREF [BREF 2009]
- Industrial gases: oxygen and nitrogen according to ecoinvent v2.2 [Ecoinvent 2010] and IFEU internal database
- Process water: ecoinvent v2.2 [Ecoinvent 2010]

For raw materials with low mass contribution LCI data from ecoinvent v2.2 [Ecoinvent 2010] are used; the most relevant materials are listed below (relevance is defined in this context as material mass per total PTA output):

- Acetic acid (< 6 %)
- Other chemicals (sum < 4 %) as sodium hydroxide, sodium carbonate, sodium formate, hydrogen, sodium hydrogen sulphite
- Catalysts (sum < 0.5 %)

Since the metal components of catalysts can have a high influence on the impact category Abiotic Depletion Potential of minerals and ores (ADP elements), their extraction was taken into account based on stoichiometric equations.

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 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 in Chapter 'Life Cycle Impact Assessment'.

Representativeness

Primary and secondary data were collected or updated according to goal and scope of this PTA Eco-profile. The data covers 79 % of the installed PTA nameplate production capacity in Europe. 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, cross-checks 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 PTA 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 the assumption 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 PTA production (bromomethane). 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

As the relevant foreground data is primary data or modelled based on primary information sources of the owner of the technology, better precision is not reachable within this goal and scope.

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 is validated and updated regularly.

Life Cycle Model

The life cycle system is modelled in Umberto 5.6, a standard software tool for LCA. The associated database integrates ISO 14040/44 [ISO 14040: 2006, ISO 14044: 2006] 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.

Calculation Rules

Vertical Averaging

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages were calculated (Figure 4). These vertical averages comprise the PTA 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, however, European average datasets were used, hence horizontal averaging was applied in these cases.

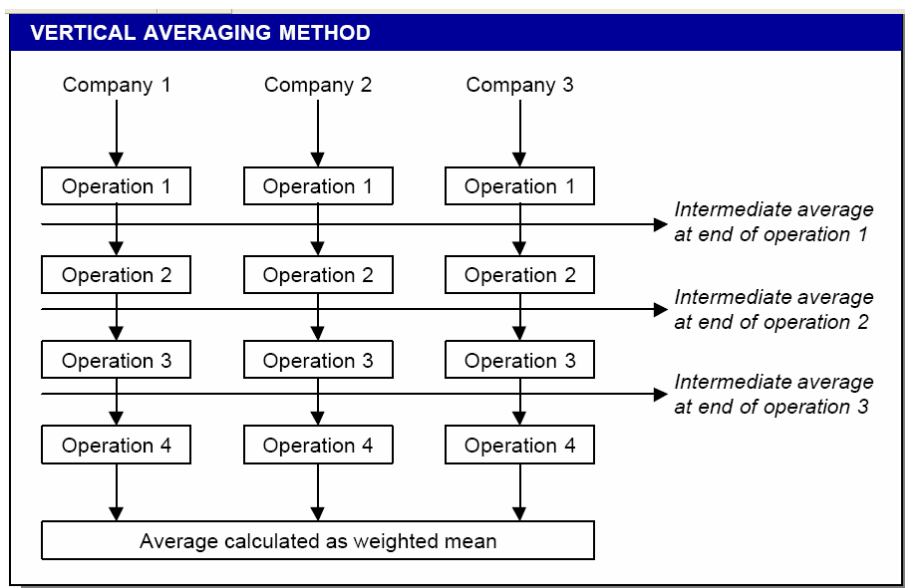


Figure 4: Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)

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 2011], 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 PTA manufacturing has no relevant by-products. Heat or steam from processes is internally used at plant sites. Therefore, allocation is not necessary for the PTA production process itself.

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 High Value Chemicals (HVC) 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 High Value Chemicals (HVC) products, 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, bioliquids 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 (LCI) Results

Formats of LCI Dataset

The Eco-profile 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 summarised below.

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) is quantified as the gross calorific value (UHV).

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

Primary Energy Demand	Value [MJ]
Energy content in PTA (energy recovery potential, quantified as gross calorific value of PTA)	19.2
Process energy (quantified as difference between primary energy demand and energy content of PTA)	36.6
Total primary energy demand (Upper heating value)	55.8
Total primary energy demand (lower heating value)	52.2

Consequently, the difference (Δ) between primary energy input and energy content in PTA output is a measure of **process energy** which 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.

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

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.82	0.041		0.82
Oil	40.83	0.892	30.70	10.13
Natural gas	11.23	0.243	0.72	10.51
Lignite	0.54	0.052		0.54
Nuclear	1.71	2.92E-06		1.71
Other non-renewable fuels	0.00			0.00
Biomass	0.21			0.21
Hydro	0.24			0.24
Solar	0.04			0.04
Geothermics	0.00			0.00
Wind	0.13			0.13
Other renewable fuels	0.00			0.00
Sub-total renewable	0.6	0.0	0.0	0.6
Sub-total Non-renewable	55.1	1.2	31.4	23.7
Total	55.8	1.2	31.4	24.3

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

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	0.6	1.1%
Non-renewable energy resources	55.1	98.9%
Total	55.8	100.0%

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

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

Type of useful energy in process input	Value [MJ]
Electricity	0.94
Thermal energy, heat	2.54
Thermal energy, cooling	1.33
Total (for selected key process)	4.81

Water Consumption

Table 5 shows the water consumption for the PTA production process (foreground process only!) whereas Table 6 shows the water consumption along the total process chain from cradle to gate.

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

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	0.0	0.0	0.0
River/canal	0.9	25.2	26.1
Sea	0.0	0.0	0.0
Unspecified	1.1	16.1	17.2
Well	0.3	0.1	0.4
Totals	2.3	41.3	43.6

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

Source	Process water [kg]	Cooling water [kg]	Total [kg]
Public supply	0.0	0.0	0.0
River/canal	0.9	26.3	27.3
Sea	0.0	3.4	3.4
Unspecified	2.4	38.5	40.9
Well	0.3	0.3	0.6
Totals	3.6	68.6	72.1

Air Emission Data

Table 7 shows a few selected air emissions for the PTA production process (foreground process only!) which are commonly reported and used as key performance indicators.

Table 7: Selected air emissions of the foreground processes (PTA production including on-site utilities) per 1 kg of product

Air emissions	kg
Carbon dioxide, fossil [kg]	0.422
Carbon monoxide (CO) [kg]	1.03E-03
Xylenes [kg]	3.87E-05
Non-methane volatile organic compounds (NMVOC, incl. xylenes) [kg]	3.97E-04
Bromomethane (Methyl bromide) [kg]	3.09E-05
Sulphur dioxide (SO ₂) [kg]	1.68E-04
Nitrogen oxides (NO _x) [kg]	4.01E-04
Particulate matter ≤ 10 µm [kg]	1.99E-05

Wastewater Emissions

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

Table 8: *Selected water emissions of the foreground processes (PTA production including on-site utilities) per 1 kg of PTA*

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	2.90E-05
Chemical oxygen demand (COD)	2.11E-04
Total organic carbon (TOC)	9.20E-05
Chloride, ion	1.75E-03
Sodium, ion	2.98E-04
Sulphate	5.27E-04

Solid Waste

Table 9 shows the solid waste generated from the PTA production process before treatment (foreground process only!) whereas Table 10 shows the solid waste generated along the total process chain from cradle to gate after waste treatment leaving the system.

Table 9: *Solid waste generation of the PTA production process (before treatment) by type and destination per 1 kg of PTA*

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	1.5E-03	8.9E-05	2.7E-04	1.9E-03	3.7E-03
Hazardous	4.7E-05	3.7E-04	3.7E-05	0.0E+00	4.6E-04
Unspecified	0.0E+00	1.1E-05	8.4E-04	0.0E+00	8.5E-04
Total	1.5E-03	4.7E-04	1.1E-03	1.9E-03	5.0E-03

Table 10: *Solid waste generation of the total process chain (cradle-to-gate, after treatment) by type and destination per 1 kg of PTA*

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous			1.7E-03		1.7E-03
Hazardous			1.9E-04		1.9E-04
Unspecified			4.0E-03		4.0E-03
Total			6.0E-03		6.0E-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 2012]. '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 11: Abiotic Depletion Potential per 1 kg PTA

Natural resources	Value
Abiotic Depletion Potential (ADP). elements [kg Sb eq]	2.24E-07
Abiotic Depletion Potential (ADP). fossil fuels [MJ]	49.7

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 12: Global Warming Potential (100 years) per 1 kg PTA

Climate change	kg CO ₂ eq.
Global Warming Potential (GWP)	1.56

Acidification

The Acidification Potential (AP) is quantified according to HAUSCHILD 1998 with updated characterisation factors of CML [CML 2012].

Table 13: Acidification Potential per 1 kg PTA

Acidification of soils and water bodies	g SO ₂ eq.
Acidification Potential (AP)	4.87

Eutrophication

The Eutrophication Potential (EP) is calculated according to HEIJUNGS 1992 with updated characterisation factors of CML [CML 2012].

Table 14: Eutrophication Potential per 1 kg PTA

Eutrophication of soils and water bodies	g PO ₄ ³⁻ eq.
Eutrophication Potential (EP), terrestrial	0.35
Eutrophication Potential (EP), aquatic	0.68
Eutrophication Potential (EP), total	1.03

Ozone Depletion

The calculation of Ozone Depletion Potential (ODP) is based on characterisation factors of the World Meteorological Organisation [WMO 2011]. 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 PTA (about 97 %). Bromomethane is an unwanted side product of the xylene oxidation reaction. It has to be noted that only two of five production units reported emissions of bromomethane even though this emission is inevitably occurring during PTA production. Bromomethane emissions can be greatly reduced through either catalytic oxidation or regenerative thermal oxidation of the waste gases followed by scrubbing.

Table 15: Ozone Depletion Potential per 1 kg PTA

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	0.0210

Summer Smog

The Photochemical Ozone Creation Potential (POCP) is quantified according to JENKIN 1999 and DERWENT 1998

with updated characterisation factors of CML [CML 2012]. 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 NMVOC. Thus, the contribution of NMVOC to POCP is 80 % (1.48 g Ethene eq./kg PTA).

Table 16: Photochemical Ozone Creation Potential per 1 kg PTA

	g Ethene eq.
Photochemical Ozone Creation Potential	1.866

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 17 are based on works of DE LEEUW 2002 and HELDSTAB 2003 for NMVOC.

Table 17: *PM10 characterisation factors of air emissions according to De Leeuw 2002 and Heldstab 2003*

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 18: *Particulate matter emissions per 1 kg PTA*

Particulate matter		
Particulate matter ≤ 10 µm (direct emissions)	0.22	g PM10 eq.
Particulate matter ≤ 10 µm, secondary	3.87	g PM10 eq.
Particulate matter ≤ 10 µm, total	4.09	g PM10 eq.
Total particulate matter	4.32	g

Dominance Analysis

Table 19 shows the main contributions to the results presented above. In this context, foreground process refers to the PTA production itself, including heat exchangers, compressors, flares, as well as on-site utilities like water preparation and wastewater treatment. Expenses and emissions concerning electric and thermal (including on-site generation of compressed air and nitrogen) energy production for the foreground process are treated separately. The sections "p-Xylene Production" and "Acetic Acid Production" refer to the production of the respective precursors including their pre-chains from the extraction of fossil resources to gate. Other raw materials include catalysts, solvents or additives and their pre-chains. Transport includes the transport of all the materials directly fed to the foreground process. Disposal refers to the waste treatment and the transport of wastes to the respective treatment facility.

The production of p-xylene is highly dominant in most of the analysed environmental impact categories. For Total Primary Energy Demand, Abiotic Depletion Potential of fossil resources (ADP fossil), Acidification Potential (AP), and emissions of particles ≤ 10µm (PM10), more than 70 % of the impact is caused by p-xylene production and the related upstream processes. The use of high quality data especially for the p-xylene production is therefore decisive to the environmental profile of PTA.

The Abiotic Depletion Potential of minerals and metal ores (ADP elements) is dominated by "other raw materials" (more than 80 %). The production of cobalt and manganese used as catalysts is the main contributor to this value (with about 92 %).

Concerning the Global Warming Potential (GWP), p-xylene production is also dominating with about 60 %, but energy production (electrical and thermal) for the PTA process and the PTA process itself contribute a significant share of about 30 % to GWP.

Table 19: Dominance analysis of impacts per 1 kg PTA

	Total Pri- mary En- ergy	ADP Ele- ments	ADP Fossil	GWP	AP	EP	ODP	POCP	PM10
	[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.]
Foreground process (PTA production)	0.0%	0.0%	0.0%	11.6%	0.9%	4.2%	97.2%	25.2%	1.3%
Electricity for foreground processes	2.9%	1.0%	1.6%	10.7%	5.4%	3.2%	0.3%	0.8%	6.1%
Thermal energy for foreground processes	9.1%	0.7%	9.1%	7.2%	2.1%	1.8%	0.2%	1.5%	2.9%
p-Xylene production	79.9%	10.8%	82.9%	60.5%	77.1%	72.8%	1.8%	65.2%	75.6%
Acetic Acid production	5.2%	6.7%	4.7%	5.1%	5.9%	13.4%	0.2%	5.8%	5.6%
Other raw materials	0.6%	79.1%	0.4%	1.1%	2.4%	2.3%	0.1%	0.6%	2.2%
Transport of raw materials	2.2%	1.1%	1.2%	3.5%	6.1%	2.4%	0.2%	0.9%	6.1%
Waste treatment	0.0%	0.0%	0.0%	0.3%	0.1%	0.1%	0.0%	0.0%	0.1%
Total	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%

The Eutrophication Potential (EP) is highly dominated by the p-xylene production and its pre-chain (more than 70 %). Acetic acid production, however, with high emissions of phosphate contributes more than 13 % to this indicator.

The Ozone Depletion Potential (ODP) of PTA is almost exclusively caused by direct emissions of bromomethane (methyl bromide) from the PTA production process.

The Photochemical Ozone Creation Potential (POCP) is dominated by the p-xylene production (about 66 %), and by the PTA production (about 25 %). Besides emissions of not further specified NMVOC (for whom a conservative impact factor of 1 g ethylene eq./kg NMVOC was used) the p-xylene production contributes high sulphur dioxide and carbon monoxide emissions resulting from the high primary energy use. The main contribution of the PTA foreground process is caused by NMVOC and xylene emissions.

Transport of raw materials to the PTA production site and treatment of wastes of PTA production have comparably low contributions to all of the impact categories.

Comparison of the present Eco-profile with its previous version (2005)

Table 20 compares the present results with the previous version of the Eco-profile of 2005. It has to be noted, that the previous Eco-profile was calculated with data referring to the year 1999. Production efficiencies and energy mixes as well as provenance mixes of fossil resources have changed significantly during the last decade. Furthermore, the underlying data set concerning p-xylene production (with its high influence on the impact factors shown in the preceding section) was updated recently, showing differences from the Eco-profile of p-xylene from 2005 which was used for the previous Eco-profile of PTA (see PLASTICSEUROPE 2013 for details). These facts have to be kept in mind when comparing the results of the current Eco-profile with its previous version.

Gross Primary Energy Demand is significantly lower than in the previous version indicating increased process efficiencies throughout the chemical industry sector, whereas the increased share of renewable energy sources (from 0.4 % to 1.1 %) reflects the changes in electricity production in Europe.

The Global Warming Potential (GWP) was calculated to be significantly lower than in the previous version. This is most likely caused by the increased efforts in reducing carbon dioxide emissions during the last decade.

For all other impact factors, a comparison is difficult since they were not included in the original report of the previous Eco-profile. The values given in Table 20 were calculated from the original LCI table using the same characterisation factors as in the current study. It has to be noted that the LCI table of the previous Eco-profile did not contain extensive information on substances with Eutrophication and Ozone Depletion Potential.

Table 20: Comparison of the present Eco-profile with its previous version [BOUSTEAD 2005]

Environmental Impact Categories	Eco-profile PTA (2005)	Eco-profile PTA (2014)	Difference
Gross primary energy from non-renewable resources [MJ]	60.34	55.14	-8.6%
Gross primary energy from renewable resources [MJ]	0.26	0.63	141.6%
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] ^{a)}	4.65×10^{-8}	2.24×10^{-7}	382.3%
Abiotic Depletion Potential (ADP), fossil fuels [MJ] ^{a)}	52.09	49.90	-4.2%
Global Warming Potential (GWP) [kg CO ₂ eq.]	2.41	1.56	-35.1%
Acidification Potential (AP) [g SO ₂ eq.] ^{a)}	10.5	4.87	-53.6%
Eutrophication Potential (EP) [g PO ₄ ³⁻ eq.] ^{a)}	0.58	1.03	79.9%
Ozone Depletion Potential (ODP) [g CFC-11 eq.] ^{b)}	n/a ^{b)}	0.021	n/a ^{b)}
Photochemical Ozone Creation Potential [g Ethene eq.] ^{a)}	1.96	1.87	-4.9%

a) Impact categories are not included in previous Eco-profile; values were calculated from LCI table using current characterisation factors.

b) not applicable: relevant substances for impact category are not listed in previous Eco-profile

Interpretation of Results

The dominance analysis in Table 19 shows that for most impact categories, the share of the processes under direct control of the PTA producer (the PTA production itself and the electrical and thermal energy production on-site) is not higher than 12 %. Exceptions are GWP and POCP with about 26-27 % and ODP with more than 97 %. Therefore, on the side of the PTA manufacturers, the main improvement options are

- increasing the process efficiency for lower energy and p-xylene input and hence an improved GWP
- continuing the work on abatement technologies for bromomethane (methyl bromide) emissions for a further reduction of ODP (best available technology today is either catalytic oxidation or regenerative thermal oxidation of the waste gases followed by scrubbing)
- improving the abatement technologies for xylene and other NMVOC emissions for a contribution to POCP reduction

It was shown in the dominance analysis, that the production of p-xylene including the whole upstream chain of crude oil and natural gas extraction and processing, the refinery processes, and the steam cracking process are highly dominant for most of the impact categories. Therefore, limitations of this study are mainly due to the uncertainties of the background datasets used.

Review

Review Summary

The subject of this critical review is the development of the Eco-profile for the European PTA production commissioned by the Committee of PET manufacturers in Europe (CPME). PTA is an important precursor for PET manufacturing.

The review process included various meetings between the LCA practitioner and the reviewer, which included a model and database review and spot checks of data and calculations. The final Eco-profile report was reviewed by Mike Neal of CPME and the reviewer. All questions and recommendations were discussed with the LCA practitioner, and the report was adapted and revised accordingly.

Primary industry data were collected for the foreground process which is basically the PTA production step itself and partly on-site energy generation, while background process data were sourced from Ecoinvent as well as specific data sources from the LCA practitioner (e.g. updated country-specific electricity grid mixes). Primary industry data was collected from 5 European PTA producers which lead to an overall representativeness of 79% of the installed European PTA production capacity.

A critical aspect of the study is that for most result indicators of the investigated product, main contributions originate from the background system (e.g. refinery, steam cracking, average p-xylene production in Europe) which is based mainly on literature data and not on primary industry data. Since these processes have a high impact on the overall results, a sound LCI analysis based on industry data of the upstream processes of PTA production is desirable for achieving lower uncertainties and higher quality of the results. However, at the moment, the resulting dataset is considered best available data and good quality with respect to the goal and scope.

The LCA practitioner has 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 PTA production in Europe.

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References

- APPE 2012 Association of Petrochemicals Producers in Europe, Personal Communication, April 2012.
- BORKEN 1999 Borken, J., Patyk, A., Reinhardt, G.A. 1999. Basisdaten für ökologische Bilanzierungen. Einsatz von Nutzfahrzeugen in Transport, Landwirtschaft und Bergbau (Basic data for life cycle assessments: Use of commercial vehicles in transport, agriculture, and mining; in German). Vieweg Verlag, Braunschweig/Wiesbaden, Germany.
- BOUSTEAD 2005 Boustead, I., Eco-profiles of the European Plastics Industry: Terephthalic Acid, Plastics Europe, March 2005
- BREF 2003 European Integrated Pollution Prevention and Control Bureau (EIPPCB) of the European Commission's Joint Research Centre (JRC): Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry, February 2003
- BREF 2009 European Integrated Pollution Prevention and Control Bureau (EIPPCB) of the European Commission's Joint Research Centre (JRC): Reference Document on Best Available Techniques in Energy Efficiency, February 2009
- BREF 2012 European Integrated Pollution Prevention and Control Bureau (EIPPCB) of the European Commission's Joint Research Centre (JRC): Draft Reference Document on Best Available Techniques for Mineral Oil and Gas Refineries, March 2012
- CML 2012 CML - Institute of Environmental Sciences: Impact assessment characterisation factors, version 4.1. CML, Leiden, October, 2012
→ <http://www.leidenuniv.nl/interfac/cml/ssp/index.html>
- DE LEEUW 2002 De Leeuw, F.A.A.M., 2002. A set of emission indicators for long-range transboundary air pollution. *Environmental Science & Policy* 5, 135-145.
- DERWENT 1998 Derwent, R.G., Jenkin, M.E., Saunders, S.M., Pilling, M.J. 1998. Photochemical ozone creation potentials for organic compounds in Northwest Europe calculated with a master chemical mechanism. *Atmospheric Environment* 32, 2429-2441.
- DERWENT 2006 Derwent, R., Simmonds, P., O'Doherty, S., Manning, A., Collins, W., Stevenson, D. 2006. Global environmental impacts of the hydrogen economy. *International Journal of Nuclear Hydrogen Production and Application* 1, 57-67.
- ECOINVENT 2010 Life cycle inventory database ecoinvent v2.2. Ecoinvent Centre, St. Gallen, 2010.
→ <http://www.ecoinvent.org>
- ECOTRANSIT 2011 IFEU Heidelberg, Öko-Institut, IVE/RMCON, 2011. EcoTransIT World - Ecological Transport Information Tool for Worldwide Transports.
- EUROSTAT 2013 Energy – Yearly statistics 2011. Eurostat, Luxembourg, 2013
→ <http://epp.eurostat.ec.europa.eu/portal/page/portal/eurostat/home>
- ETS 2009 Ecofys et al.: Methodology for the free allocation of emission allowances in the EU ETS post 2012 - Sector report for the chemical industry, 2009

EYERER 1996	Ganzheitliche Bilanzierung – Werkzeug zum Planen und Wirtschaften in Kreisläufen, 1996
FRANCK 1987	H.-G. Franck, J. W. Stadelhofer: Industrielle Aromatenchemie. Rohstoffe, Verfahren, Produkte, Springer, 1987
GUINÉE ET AL. 2002	Guinée, J.B., Gorée, M., Heijungs, R., Huppes, G., Kleijn, R., de Koning, A., van Oers, L.F.C.M., Wegener Sleeswijk, A., Suh, S., Udo de Haes, H.A., de Bruijn, H., van Duin, R., Huijbregts, M.A.J., 2002. Handbook on Life Cycle Assessment: An operational Guide to the ISO Standards. Kluwer Academic Publishers, Dordrecht, The Netherlands.
HAUSCHILD 1998	Hauschild, M, Wenzel, H.: Environmental Assessment of products. Volume 2: Scientific background. Chapman & Hall, London, 1998
HBEFA 2010	INFRAS AG, Handbook of Emission Factors for Road Transport (HBEFA) version 2.1, January 2010. → http://hbefa.net
HEIJUNGS 1992	Heijungs, R., J. Guinée, G. Huppes, R.M. Lankreijer, H.A. Udo de Haes, A. Wegener Sleeswijk, A.M.M. Ansems, P.G. Eggels, R. van Duin, H.P. de Goede, 1992: Environmental Life Cycle Assessment of products. Guide and Backgrounds. Centre of Environmental Science (CML), Leiden University, Leiden.
HELDSTAB 2003	Heldstab, J., de Haan van der Weg, P., Künzle, T., Keller, M. Zbinden, R., 2003. Modelling of PM10 and PM2.5 ambient concentrations in Switzerland 2000 and 2010. Environmental Documentation No.169. Swiss Agency for the Environment, Forests and Landscape (SAEFL), Bern, Switzerland.
HISCHIER 2007	Hischier, R. 2007. Life Cycle Inventories of Packaging and Graphical Papers. ecoinvent-Report No. 11, Part III, Chapter 10.3 "Production of purified terephthalic acid (PTA)". Swiss Centre for Life Cycle Inventories, Dübendorf, Switzerland.
IFEU 2011	Lauwigi, Ch., Fehrenbach, H., October 2011: Documentation for the UMBERTO based electricity grid model created by IFEU. Institute for Energy and Environmental Research, Heidelberg, Germany. → http://ifeu.de/english/index.php?bereich=ind&seite=energieerzeugung
IPCC 2013	IPCC, 2013: Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment. Report of the Intergovernmental Panel on Climate Change. [Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M. Tignor and H.L. Miller (eds.)]. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA.
ISO 14040: 2006	ISO 14040 Environmental Management – Life Cycle Assessment – Principles and Framework. Geneva, 2006
ISO 14044: 2006	ISO 14044 Environmental management -- Life cycle assessment -- Requirements and guidelines. Geneva, 2006
ILCD 2010	European Commission (2010): ILCD Handbook – General guide for Life Cycle Assessment (LCA) – Detailed guidance

JENKIN 1999	Jenkin, M.E. and Hayman, G.D., 1999. Photochemical ozone creation potentials for oxygenated volatile organic compounds: sensitivity to variations in kinetic and mechanistic parameters. <i>Atmospheric Environment</i> 33, 1775-1293.
MEYERS 2003	Robert A. Meyers (ed.): <i>Handbook of Petroleum Refining Processes</i> , 3rd edition. 2003
NIST 2011	National Institute of Standards and Technology (NIST), NIST Chemistry Webbook, 2011, USA (webbook.nist.gov)
PLASTICSEUROPE 2011	Life Cycle Inventory (LCI) Methodology and Product Category Rules (PCR) for Uncompounded Polymer Resins and Reactive Polymer Precursors. 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). PlasticsEurope, November 2012.
PLASTICSEUROPE 2013	Eco profiles and Environmental Product Declarations of the European Plastics Manufacturers -- Benzene, Toluene, and Xylenes (Aromatics, BTX). PlasticsEurope, February 2013.
RASEEV 2003	S. Raseev: <i>Thermal and Catalytic Processes in Petroleum Refining</i> , Marcel Dekker AG, 2003
TREMODO 2009	IFEU 2009. TREMOD - Transport Emission Model: "Daten- und Rechenmodell Schadstoffemissionen aus dem motorisierten Verkehr in Deutschland 1960-2030".
ULLMANN 2010	Ullmann's Encyclopedia of Industrial Chemistry, John Wiley & Sons, Inc. , Hoboken / USA, 2010
WAUQUIER 2000	J.-P. Wauquier (Ed.), <i>Petroleum Refining 2. Separation Processes</i> , Editions Technip, 2000
WHO 2006	World Health Organization (WHO), Joint WHO / Convention Task Force on the Health Aspects of Air Pollution, 2006. Health risk of particulate matter from long-range transboundary air pollution.
WMO 2011	WMO (World Meteorological Organization), Scientific Assessment of Ozone Depletion: 2010, Global Ozone Research and Monitoring Project – Report No. 52, 516 pp., Geneva, Switzerland, 2011.

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