Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers

Aromatic Polyester Polyols (APP)
PU Europe
February 2016

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Environmental Product Declaration

Introduction

This Environmental Product Declaration (EPD) is based upon life cycle inventory (LCI) data from 2014 and the GaBi database 2014 fulfilling the requirements on 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** (PCR version 2.0, April 2011). EPDs provide environmental performance data, but no information on the economic and social aspects which would be necessary for a complete sustainability assessment. EPDs do not imply a value judgement between environmental criteria.

This EPD describes the production of aromatic polyester polyols (APP) from cradle to gate (from crude oil extraction to liquid resin at plant, i.e. APP production site output). **Please keep in mind that comparisons cannot be made on the level of the polymer material 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	PU Europe aisbl
LCA Practitioner	thinkstep AG
Programme Owner	Plastics Europe aisbl
Programme Manager, Reviewer	DEKRA Assurance Services GmbH
Number of plants included in data collection	5
Representativeness	75-85%
Reference year	2014
Year of data collection and calculation	2015
Expected temporal validity	2024
Cut-offs	No significant cut-offs
Data Quality	Good
Allocation method	Price allocation (for one of the products)

Description of the Product and the Production Process

Aromatic Polyester Polyols comprises a group of products which are polymers. Therefore neither a CAS number, nor an IUPAC name, nor a chemical formula can be stated. The following products are considered:

LUPRAPHEN (BASF)
HOOPOL (Synthesia)
TERATE (Invista)
ISOEXTER 3061 (COIM)
STEPANPOL (Stepan)

Polyester Polyols are important intermediate products for many production chains. APPs are used to manufacture polyisocyanurate (PIR) and polyurethane (PUR) rigid insulation foam, which finds extensive use in the automotive, construction, refrigeration and other industrial sectors. Other uses include flexible polyurethane foams, semi-rigid foams, and polyurethane coatings. A major part of the world's polyols production is shared by two groups of polyols, namely polyether and polyester polyols.

Production Process

Aromatic polyester polyols result from the polycondensation from a variety of potential input materials such as di- or trifunctional polyols, e.g. diethylene glycol and aromatic anhydrides, e.g. phthalic anhydrides. Also the the production technology can differ from producer to producer.
The reference flow, to which all data given in this EPD refer, is 1 kg of average aromatic polyester polyols (APP).

Data Sources and Allocation

The main data source is a primary data collection from European producers of APP, providing site-specific gate-to-gate production data for processes under operational control of the participating companies: 5 producers with 5 plants / 6 products in 4 different European countries.

This covers more than 75-85 % of a total market of more than 100,000 t of the European APP production (EU-27) in 2014.

The data for the upstream supply chain until the precursors are taken from the database of the software system GaBi 6 [GABI 6].

All relevant background data, such as energy and auxiliary materials, is from the GaBi 6 database; the documentation is publicly available [GABI 6].

Use Phase and End-of-Life Management

Due to high resistance to light and thermal aging, as well as thermal stability of polyurethane produced with APPs, the polyurethane/polyisocyanurate (PUR/PIR, in the following the common term for both PU is applied) products are used for paints, coating materials and flame-retarded rigid foams [ULLMANN 2010]. They also may be formulated into adhesives, sealants, and elastomers.

Polyurethanes are made from polyols e.g. APPs and polyisocyanates. Typical isocyanates used include polymeric methylene diphenyl diisocyanate (PMDI) in rigid foam applications. Toluene diisocyanate (TDI) is used in flexible foam applications. Monomeric MDI is used in adhesive, coating, sealant, and elastomer applications. Flame retardants may be included in the APP batch and/or added separately during PUR production. This Eco-profile refers to APP without flame retardant additions.

When used in thermal insulation products, the use phase results in substantial energy savings of buildings / technical installations / fridges over their use phase.

Today's most important process for an end-of-life is an energy recovery of the PU material.

Most of the production waste (and some installation off-cuts) is recycled.

Environmental Performance

The tables below show the environmental performance indicators associated with the production of 1 kg APP.

Input Parameters

Indicator	Unit	Value
Non-renewable energy resources[1)]	MJ	66.79
• Fuel energy	MJ	42.04
• Feedstock energy	MJ	24.75*
Renewable energy resources (biomass)[1)]	MJ	3.27
• Fuel energy	MJ	1.63
• Feedstock energy	MJ	1.64
Abiotic Depletion Potential		
• Elements	kg Sb eq	1.05E-06
• Fossil fuels	MJ	59.5
Renewable materials (biomass) (key foreground process level)	Kg	- **
Water use (key foreground process level)	kg	5.04
• for process	kg	na
• for cooling	kg	na

[1)] Calculated as upper heating value (UHV)

na= not available – details see table 9

* since this value cannot be retrieved directly from the LCA model, it was assumed as 110% of the APP upper calorific value (assumption in accordance with several Eco-profiles since 2010)

** due to confidentiality reasons, this value cannot be communicated

Output Parameters

Indicator	Unit	Value
GWP	kg CO_2 eq	1.82
ODP	g CFC-11 eq	2.22E-07
AP	g SO_2 eq	5.59
POCP	g Ethene eq	2.04
EP	g PO_4 eq	1.10
Dust/particulate matter PM10[2)]	g PM10	1,87E-01
Total particulate matter[2)]	g	2.49E-01
Waste		
• Radioactive waste	kg	9.16E-04
• Non-radioactive waste [3)]	kg	3.23E-02

[2)] Including secondary PM10

[3)] Non-radioactive wastes include: spoil, tailings, and waste, deposited

Additional Environmental and Health Information

Not available

Additional Technical Information

The incorporated aromatic acid provides thermal stability which allows the rigid foam to pass typical building code flammability tests. The aromatic acid also provides hydrolysis resistance to the final product.

Regarding flame retardant, from the existing APP Eco-profile (results from study published in 2010) only the dataset without flame retardant is updated and presented here. Many application areas of APP require different amounts of flame retardant. Hence, the respective amounts (including its potential environmental burdens) need to be added afterwards anyways. The input of flame retardant (including its potential environmental burdens) can be easily added afterwards since it is physically mixed and does not require a chemical linkage.

Additional Economic Information

When used in thermal insulation products, APP enables substantial energy savings of buildings / technical installations / fridges over their use phase.

Information

Data Owner

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Programme Manager & Reviewer
DEKRA Assurance Service GmbH
This Environmental Product Declaration has been reviewed by DEKRA Assurance Service GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006.
Registration number: PlasticsEurope 2016-001 validation expires on 31 January 2019 (date of next revalidation review).

Programme Owner

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E-mail: info@plasticseurope.org.

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: Eco-profiles and environmental declarations – LCI methodology and PCR for un-compounded polymer resins and reactive polymer precursors (version 2.0, April 2011).

PU EUROPE
EXCELLENCE IN INSULATION

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.

PlasticsEurope Eco-profiles and EPDs represent polymer production systems with a defined output. They can be used as modular building blocks in LCA studies. However, these integrated industrial systems cannot be disaggregated further into single unit processes, such as polymerisation, 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.

PlasticsEurope Eco-profiles and EPDs are prepared in accordance with the stringent ISO 14040–44 requirements. Since the system boundary is »cradle-to-gate«, however, their respective 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 building products where PlasticsEurope 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, 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 and reactive polymer precursors**. This product category is defined »at gate« of the polymer or precursor production and is thus fully within the scope of PlasticsEurope as a federation. In some cases, it may be necessary to include one or several additives in the Eco-profile to represent the polymer or precursor »at gate«. For instance, some polymers may require a heat stabiliser, or a reactive precursor may require a flame retardant. This special case is distinguished from a subsequent compounding step conducted by a third-party downstream user (outside PlasticsEurope's core scope).

Functional Unit and Declared Unit

The default Functional Unit and Declared Unit of PlasticsEurope Eco-profiles and EPDs are (unless otherwise specified[1]):

1 kg of aromatic polyester polyols (APP)– »at gate« (production site output) representing a European industry production average with an average calorific value of 22.5 MJ and a hydroxyl value of 150-360 and aromatic content of 5-50%

Product and Producer Description

Product Description

APP is a reactive polymer precursor used for the production of polyurethane PU rigid insulation foam. Data for other components of this foam are available, especially polymeric MDI [ISOPA 2012 TDI-MDI]. APP product trade names considered in this study are the following:

BASF: LUPRAPHEN
SYNTHESIA: APP: HOOPOL
INVSTA: TERATE
COIM: ISOEXTER 3061
STEPAN: STEPANPOL® polyester polyol

As some of the considered products/brands consists of a mixture of several APP variants, specific information such as CAS no, formula and calorific value cannot always be delivered.

Production Process Description

Aromatic polyester polyols are made by polycondensation from a variety of potential input materials such as multifunctional glycols, e.g. diethylene glycol with multifunctional aromatic anhydrides and acids, e.g. phthalic anhydride, terephthalic acid, isophthalic acid. Also the production technology can differ from producer to producer.

Basically the process can be described as follows: The alcohol is first heated, then dicarboxylic acid/anhydride is added and the reaction water is removed. The amount of excess diol determines the molecular weight of the product, which also ~~and it~~ depends on the processing conditions and the type of diol. Nitrogen, carbon

[1] Exceptions can occur when reporting Eco-profiles of, for instance, process energy, such as on-site steam, or conversion processes, such as extrusion.

dioxide or vacuum is used to remove the water and to reach the aimed conversion of more than 99%. Catalysts are used reluctantly because they cannot be removed and can have an undesirable effect on the following PU reaction.

Producer Description

PlasticsEurope Eco-profiles and EPDs represent European industry averages within the scope of PU Europe and PlasticsEurope as the issuing trade federations. Hence they are not attributed to any single producer, but rather to the European plastics industry as represented by PU Europe's membership and the production sites participating in the Eco-profile data collection. The following companies contributed to provide data to this Eco-profile and EPD:

- BASF SE

  Carl Bosch Str 38
  67056 Ludwigshafen
  Germany
  http://www.basf.com

- COIM S.p.A.

  Via Ricengo 21/23
  26010 Offanengo (CR)
  Italy
  http://www.coimgroup.com

- INVISTA Polyester B.V.

  Europaweg Zuid 2a / PO Box 408
  4389 PD Ritthem / NL-4380 AK Vlissingen
  The Netherlands
  http://www.invista.com

- Stepan Deutschland GmbH

  Rodenkirchener Str. 400
  50389 Wesseling
  Germany
  http://www.stepan.com

- SYNTHESIA INTERNACIONAL S.L.U.

  C/Argent, 3 – Àrea Industrial del Llobregat
  08755 Catellbisbal (Barcelona)
  Spain
  http://www.synthesiainternacional.com/

Eco-profile – Life Cycle Inventory

System Boundaries

PlasticsEurope Eco-profiles and EPDs refer to the production of polymers as a cradle-to-gate system (see Figure 1)

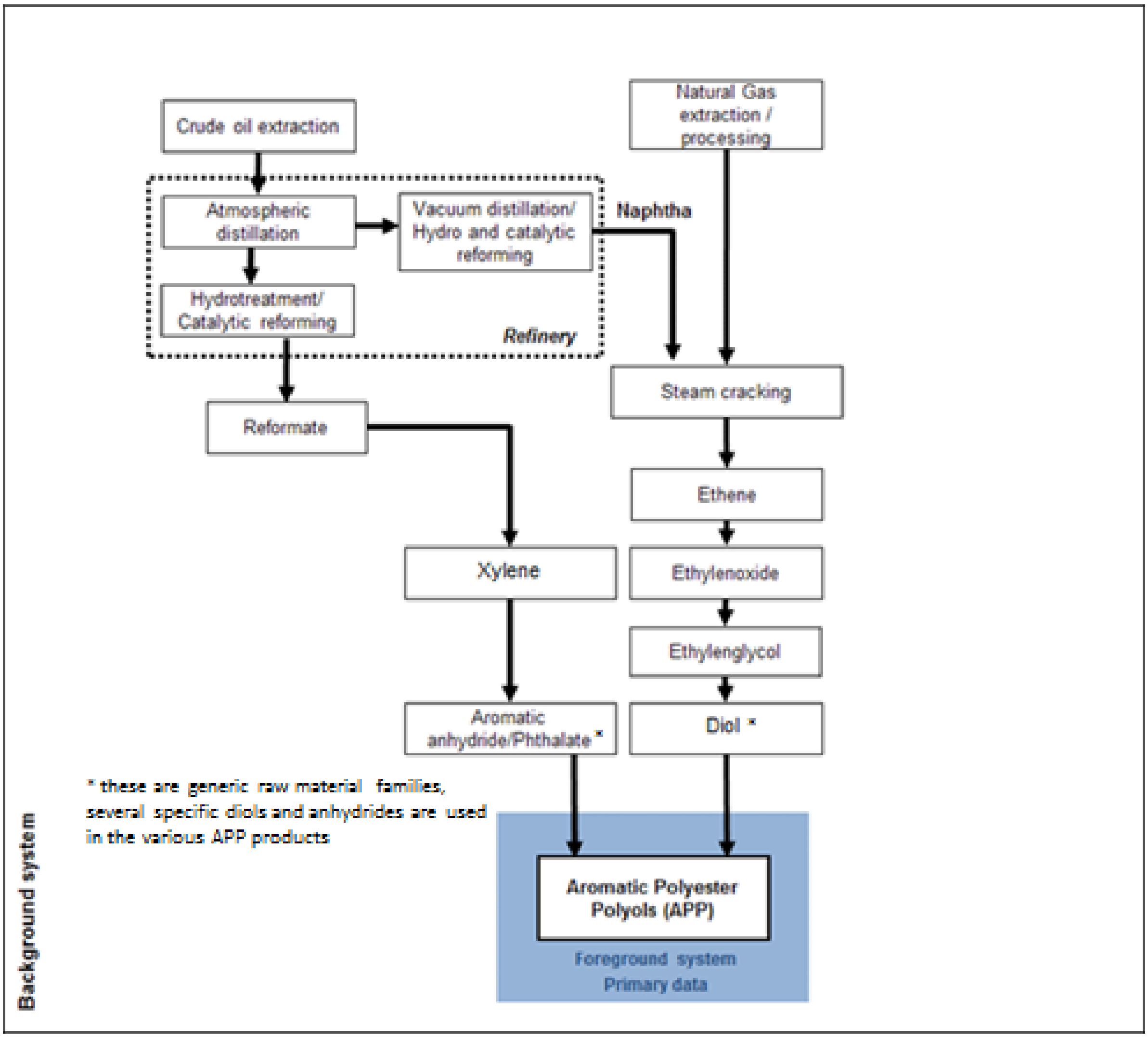


Figure 1: Cradle-to-gate system boundaries (APP)

Technological Reference

The production processes are modelled using specific values from primary data collection at site. The main data source is a primary data collection from European producers of APP, providing site-specific gate-to-gate production data for processes under operational control of the participating companies: five APP producers with five plants in four different European countries.

The data cover 75-85% [PU Europe 2015] of the European APP production (EU-27) in 2014. Primary data are used for all foreground processes (under operational control) complemented with secondary data for background processes (under indirect management control). The data for the upstream supply chain until the precursors are taken from the database of the software system GaBi 6 [GaBi 6].

Temporal Reference

The LCI data for production is collected as 12 month averages representing the year 2014, to compensate seasonal influence of data. Background data have reference years between 2011 and 2013 for electricity and thermal energy processes. The dataset is considered to be valid until substantial technological changes in the production chain occur. In view of the latest technology development, the overall reference year for this Eco-profile is 2014, with a maximum temporal validity until 2024 for the foreground system.

Geographical Reference

Primary production data for APP production are from five different European suppliers. The inventories for the precursors and the energy supply are adapted according to site specific (i.e. national) conditions. Inventories for the group of "Other chemicals", used in smaller amounts, refer to European conditions or geographical conditions as the datasets are available. Therefore, the study results are intended to be applicable within EU boundaries: adjustments might be required if the results are applied to other regions. APP imported into Europe is not considered in this Eco-profile.

Cut-off Rules

In the foreground processes all relevant flows are considered, with no cut-off of material and energy flows. According to the GaBi database [GABI 6], used in the background processes, at least 95% of mass and energy of the input and output flows are covered and 98% of their environmental relevance (according to expert judgment) are considered, hence an influence of cut-offs less than 1% on the total is expected. Transports for the main input materials (Diol/Triol, Phthalates) were considered. The contribution of transport of small material proportions is expected to be less than 1%; hence the transports for minor input amounts are excluded.

Data Quality Requirements

Data Sources

Eco-profiles and EPDs developed by PU Europe use 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 PU Europe (see Producer Description).
The data for the upstream supply chain are taken form the life cycle database of the software system GaBi [GABI 6]. Most of the background data used is publicly available and public documentation exists.

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 was sourced from the most important APP producers in Europe in order to generate a European production average. The environmental contributions of each process to the overall LCI results are included in the Chapter 'Life Cycle Impact Assessment'.

Representativeness

The participating companies represent 75-85% of the European APP production volume in 2014. This figure refers to an educated estimate of PU Europe and the participating parties of this study. [PU Europe 2015]. The selected background data can be regarded as representative for the intended purpose.

Consistency

To ensure consistency, only primary data of the same level of detail and background data from the GaBi 6 databases [GABI 6] are used. While building up the model, cross-checks ensure the plausibility of mass and energy flows. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in the foreground and background systems. In addition to the external review, an internal independent quality check is performed (see 'Internal Independent Quality Assurance Statement').

Reliability

Data of foreground processes provided directly by producers are predominantly measured. Data of relevant background processes are measured at several sites – alternatively, they are determined from literature data, or estimated for some flows, which usually are reviewed and quality checked.

Completeness

Primary data used for the gate-to-gate production of APP covers all related flows in accordance with the above cut-off criteria. In this way all relevant flows are quantified and data is considered complete. The elementary flows covered in the model enable the impact assessment of all selected impact categories. Waste treatment is included in the model, so that only elementary flows cross the system boundaries.

Precision and Accuracy

As the relevant foreground data is primary data, or modelled based on primary information sources of the owners of the technologies, precision is deemed appropriate to the goal and scope.

Reproducibility

Reproducibility is given for internal use since the owners of the technologies provided the data under confidentiality agreements. Key information is documented in this report, and data and models are stored in the GaBi 6 software 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, full and detailed reproducibility will not be possible for confidentiality reasons. However, experienced practitioners could reproduce suitable parts of the system as well as key indicators in a certain confidence range.

Data Validation

The data on production collected by the project partners and the data providing companies are validated in an iterative process several times. The collected data are validated using existing data from published sources or expert knowledge. The background information from the GaBi database is updated regularly and continuously validated.

Life Cycle Model

The study is performed with the LCA software GaBi 6 [GABI 6]. The associated database integrates ISO 14040/44 requirements. Due to confidentiality reasons details on software modelling and methods used cannot be shown here. However, provided that appropriate confidentiality agreements are in place, the model can be reviewed in detail; an external independent review has been conducted to this aim. The calculation follows the vertical calculation methodology (see below).

Calculation Rules

Vertical Averaging

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages are calculated (Figure 2).

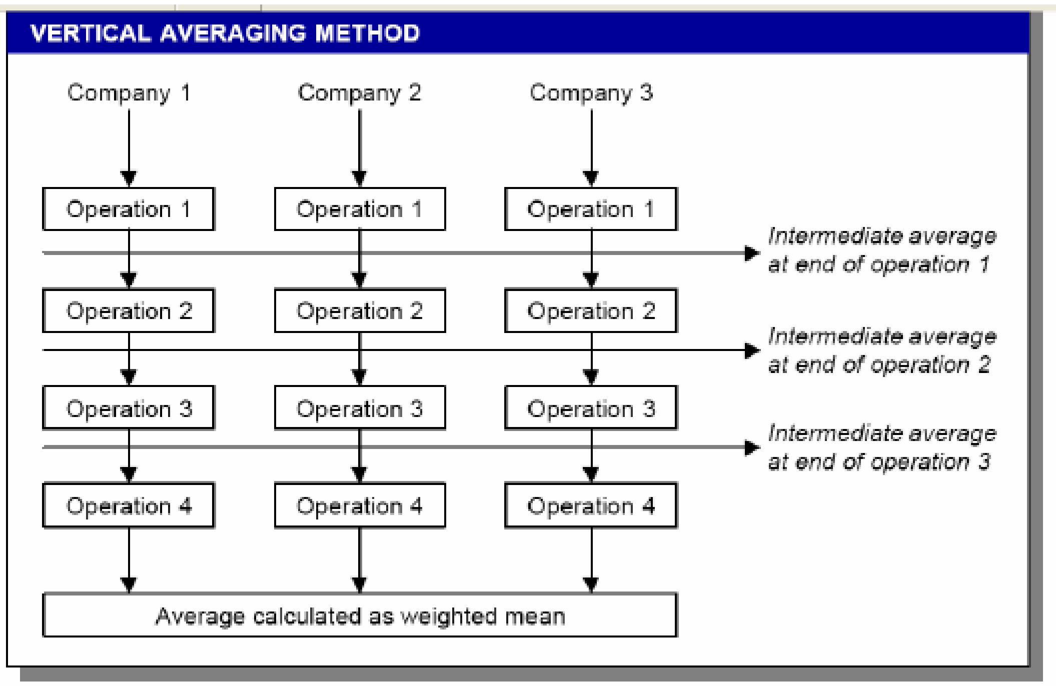


Figure 2: Vertical Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI (European Council for Plasticisers and Intermediates, 2001)

Due to the fact that various APP products exist based on various input materials and production technologies, detailed discussions were held on whether it is possible to provide Eco-profile data for different types of APP products. However, out of the following reasons, only one aggregated dataset for one average APP product is presented:

- A desired performance of an APP can be achieved with different production technologies and different combinations of input materials.
- Similarly, for given application areas of APP, input materials and production technologies are basically exchangeable.
- As soon as Eco-profiles for specific APP formulations are revealed, confidentiality of company-specific data may not be ensured. In addition, environmental performance results of specific APP formulations may favour a particular manufacturer which defeats the purpose of this Eco-profile initiative.

- It is common practice that clients of APP are switching suppliers;

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. Wherever possible, allocation should be avoided by expanding the system to include the additional functions related to the co-products. Often, however, avoiding allocation is not feasible in technical reality, as alternative stand-alone processes do not exist or even 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.

Foreground system

In some companies' information, output material with deviations from the required specification is reported. If these materials show significant differences and are sold at a different price levels (like the condensate), a price allocation is used based on the sales price ratio of the main product and co-product. In case of material declared as off-grade sent to recovery, neither further environmental burden nor credits are given to the modelled system (< 1% of total production). If the co-products are reused in the same process, then the output is looped back as an input.

When recycled material is reported as input to the system (1% of the average APP) the input dataset used is modelled using the recycled content approach: scrap inputs to the recycled product system are modelled as being free of any primary material burden, only burden for the recycling process are taken into account.

Background system

In the refinery operations, co-production is addressed by applying allocation based on mass and net calorific value [GABI 6]. The chosen allocation in downstream petrochemicals is based on several sensitivity analyses, which were reviewed by petrochemical experts. Materials and chemicals needed are modelled using the allocation rule most suitable for the respective product (mass, energy, exergy, economic). For further information on specific product see documentation on www.gabi-software.com .

Life Cycle Inventory (LCI) Results

Formats of LCI Dataset

The Eco-profile is provided in four 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)
- As LCI in GaBi format (www.gabi-software.com)

Key results are summarised below.

Energy Demand

As a key indicator on the inventory level, the **primary energy demand** (system input) of 70.06 MJ/kg 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).

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 about 22.50 MJ/kg for APP.

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

Primary Energy Demand	Value [MJ]
Energy content in polymer (energy recovery potential, quantified as gross calorific value of polymer)	22.50
Process energy (quantified as difference between primary energy demand and energy content of polymer)	47.56
Total primary energy demand	**70.06**

Consequently, the difference (Δ) between primary energy input and energy content in polymer output is a measure of **process energy** which may be either dissipated as waste heat or recovered for use within the system boundaries.

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. Note that some feedstock input may still be valorised as energy; furthermore, process energy requirements may also be affected by exothermal or endothermal reactions of intermediate products. Hence, there is a difference between the feedstock energy input and the energy content of the polymer (measurable as its gross calorific value). Considering this uncertainty of the exact division of the process energy as originating from either fuels or feedstocks, as well as the use of average data (secondary data) in the modelling with different country-specific grades of crude oil and natural gas, the feedstock energy is presented as approximate data.

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

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	1.62	0.06		1.62
Oil	38.16	0.85	14.40	9.75
Natural gas	23.09	0.47	8.71	5.90
Lignite	1.61	0.12		1.61
Peat	0.00	0.00		0.00
Nuclear	2.31	5.12E-06		2.31
Biomass	0.00	0.00	0.00	0.00
Hydro	0.25			0.25
Solar	2.50	0.05	1.64	0.86
Geothermics	6.39E-03			6.39E-03
Waves	8.95E-13			8.95E-13
Wood	0.00			0.00
Wind	0.52			0.52
Other renewable fuels	0.00			0.00
Sub-total renewable	**3.27**	**0.00**	**1.64**	**1.63**
Sub-total Non-renewable	**66.79**	**1.50**	**23.11**	**43.68**
Total	**70.06**	**1.50**	**24.75**	**45.31**

Table 3 shows that nearly all of the primary energy demand is from non-renewable resources. Since the focus scope of PU Europe and their member companies is the polymer production, Table 4 analyses the types of useful energy inputs in the reaction process leading to APP: electricity has a minor contribution compared to thermal energy (heat). This represents the share of the energy requirement that is under operational control of the polymer producer (Figure 3). Accordingly, Table 5 shows that the majority (95.3%) of the primary energy demand is accounted for by upstream (pre-chain) processes. Finally, Table 6 provides a more detailed overview of the key processes along the production system, their contribution to primary energy demand and how this is sourced from the respective energy resources. This puts the predominant contribution of the production into perspective with the precursors (»precursors and process«). In order to analyse these upstream operations more closely, please refer to the Eco-profiles and GaBi documentations of the respective precursors.

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

Fuel/energy input type	Value [MJ]	%
Renewable energy resources	3.27	4.7%
Non-renewable energy resources	66.79	95.3%
Total	**70.06**	**100.0%**

Table 4: Analysis by type of useful energy (production – key foreground process level) per 1 kg APP

Type of useful energy in process input	Value [MJ]
Electricity	0.38
Heat, thermal energy	3.35
Other types of useful energy (relevant contributions to be specified)	0.00
Total (for selected key unit process)	**3.73**

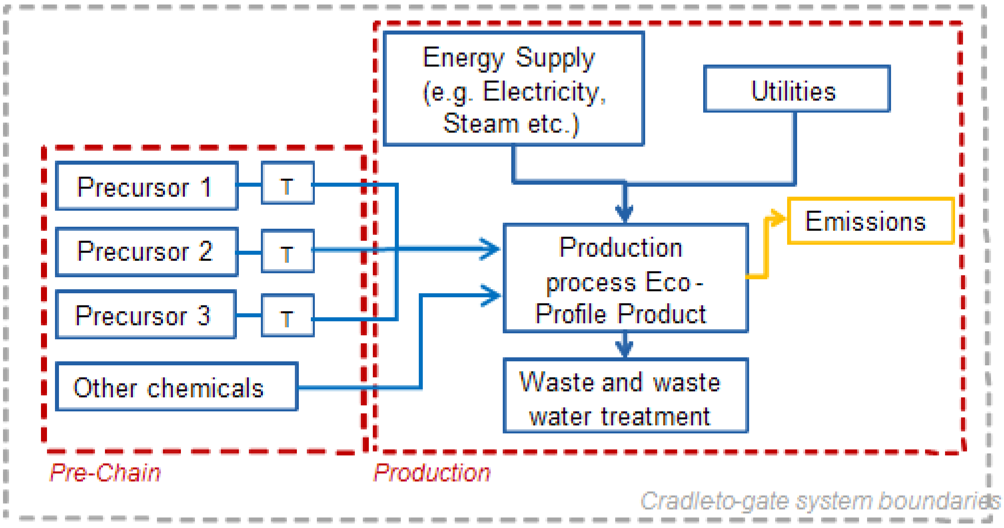
Table 5: Contribution to primary energy demand (dominance analysis) per 1 kg APP

Contribution to Primary Energy per segment	Value [MJ]	%
Production (electricity, steam, unit process, utilities[1)], waste treatment)	3.28	4.7%
Pre-chain[2)]	66.78	95.3%
Total	**70.06 ***	**100.0%**

[1)] Including water, catalyst, nitrogen, compressed air
[2)]Incl. raw materials, e.g. Diols, Phthalates, etc.

Table 6: Contribution of life cycle stages to total primary energy demand (gross calorific values) per 1 kg APP, see Figure 3

Total Primary Energy [MJ]	Precursors & Process	Other Chemicals	Utilities	Electricity	Thermal Energy	Transport	Process Waste Treatment
Coal	1,32E+00	6,36E-02	1,11E-02	2,20E-01	4,13E-03	1,28E-03	1,12E-03
Oil	3,69E+01	8,30E-01	6,61E-03	3,66E-02	5,68E-03	3,72E-01	1,76E-03
Natural gas	2,04E+01	7,76E-01	1,67E-02	3,14E-01	1,59E+00	3,27E-02	-4,03E-03
Lignite	1,35E+00	5,91E-02	8,80E-03	1,85E-01	3,36E-03	9,30E-04	8,36E-04
Peat	3,84E-03	4,84E-05	7,89E-05	3,86E-05	7,88E-06	1,27E-05	7,07E-06
Nuclear	2,04E+00	5,36E-02	1,38E-02	1,97E-01	3,91E-03	1,79E-03	5,94E-04
Biomass	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Hydro	2,16E-01	6,43E-03	2,15E-03	2,93E-02	6,75E-04	3,92E-04	4,97E-05
Solar	7,21E-01	1,64E+00	4,56E-03	1,15E-01	2,10E-03	1,39E-02	1,22E-04
Geothermics	5,74E-03	1,61E-04	8,94E-05	3,47E-04	3,09E-05	1,80E-05	7,59E-06
Waves	7,47E-13	2,97E-14	4,11E-15	1,12E-13	1,96E-15	3,16E-16	1,23E-16
Wood	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Wind	4,10E-01	1,57E-02	3,22E-03	8,49E-02	1,42E-03	2,82E-04	-1,01E-04
Other renewable fuels	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Total	**6,33E+01**	**3,45E+00**	**6,72E-02**	**1,18E+00**	**1,61E+00**	**4,23E-01**	**3,66E-04**



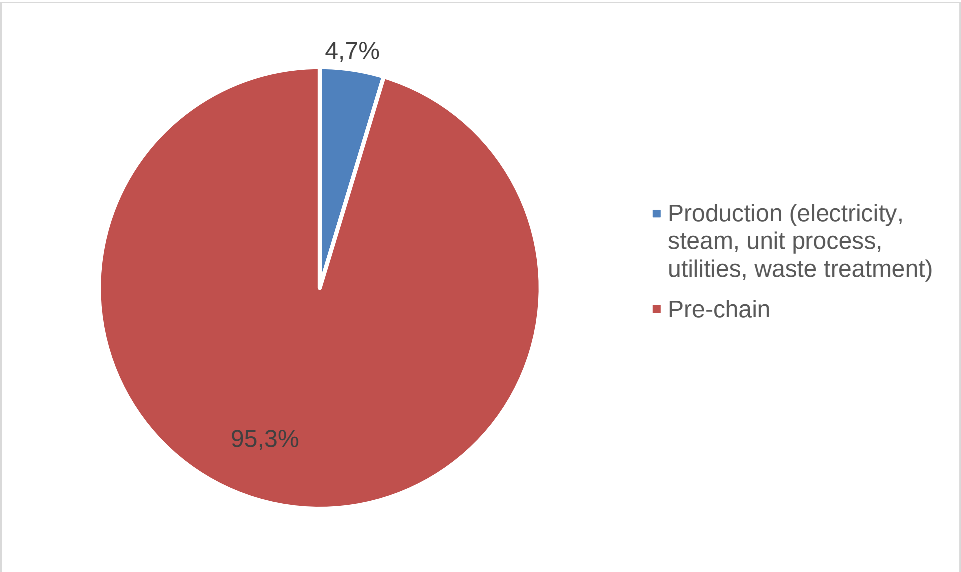


Figure 3: Contribution to primary energy demand per segment

Water Consumption

Table 7 shows the water use at cradle-to-gate level. Water use (incl. fresh- and seawater; blue- and green water) equals the measured water input into a product system or process. Water use is determined by total water withdrawal (water abstraction).

Table 7: Water use (fresh- and seawater; blue- and greenwater) table per 1 kg APP (cradle-to-gate)

Input	Value [kg]
Water (ground water)	29.99
Water (lake water)	32.27
Water (rain water)	92.57
Water (river water)	1082.73
Water (sea water)	7.45
Water (fossil groundwater)	0.00
Overall water use [kg]	**1245.00**

Table 8 provides the corresponding freshwater part in the water balance. Freshwater is naturally occurring water on the Earth's surface in ponds, lakes, rivers and streams, as ice, and underground as groundwater in aquifers and underground streams. The term specifically excludes seawater and brackish water. Blue water refers to surface and groundwater used.

Table 8: Freshwater (blue water not including rain water) use table per 1 kg APP (cradle-to-gate)

Input	**Value [kg]**
Water (ground water)	29.99
Water (lake water)	32.27
Water (river water)	1082.73
Water (fossil groundwater)	0.00
Total fresh water use [kg]	**1144.98**

Output	**Value [kg]**
Water (river water from technosphere, cooling water)	38.53
Water (river water from technosphere, turbined)	1068.59
Water (river water from technosphere, waste water)	4.52
Water (lake water from technosphere, cooling water)	0.00
Water (lake water from technosphere, turbined)	0.00
Water (lake water from technosphere, waste water)	0.00
Total fresh water release from technosphere (degradative use) [kg]	**1111.63**
Total fresh water consumption (blue water)	**33.35**

Figure 4: Total fresh water use (input) / water release (output) and water consumption (APP)

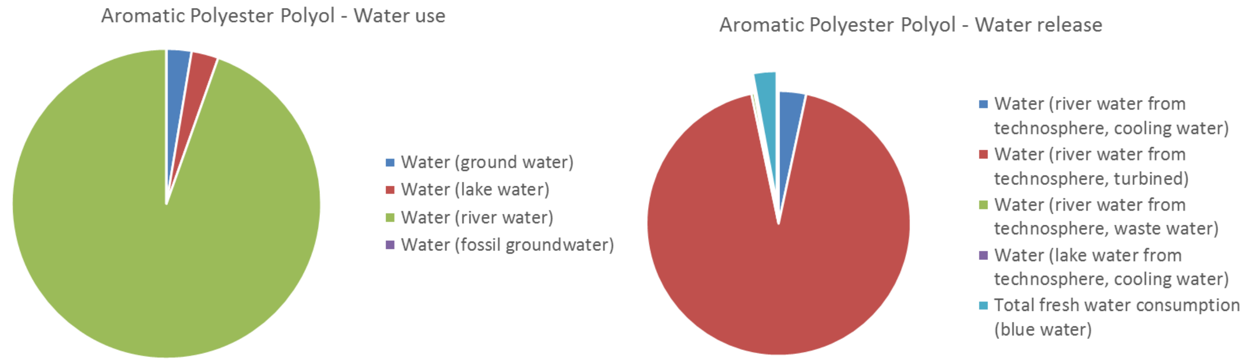


Table 9 shows the water balance at key foreground process level.
At key foreground process level the water output is slightly higher than the water input: this is due to rain water going to wastewater as well as water generated during esterification reaction.

Table 9: Water balance table per 1 kg APP (key foreground process level)

Input	**Value [kg]**
Water (cooling water)[2]	1.02E-03
Water (process water)	3.58E-01
Water (deionised)	1.87E-02
Water (tap water)	1.39E-01
Water (ground water)	0.00E+00
Water (river water)	0.00E+00
Water (sea water)	4.52E+00
Total water input	**5.04E+00**
Output	**Value [kg]**
Water vapour	4.24E-02
Water (waste water, untreated) to WWTP	5.86E-01
Water direct released to the environment without WWTP	
Water (river water from technosphere, cooling water)	0.00E+00
Water (river water from technosphere, turbined)	0.00E+00
Water (river water from technosphere, waste water)	0.00E+00
Water (sea water from technosphere, cooling water)	4.52E+00
Water (sea water from technosphere, turbined)	0.00E+00
Water (sea water from technosphere, waste water)	0.00E+00
Water (lake water from technosphere, cooling water)	0.00E+00
Water (lake water from technosphere, turbined)	0.00E+00
Total water output	**5.15E+00**

Air Emission Data

Table 10 shows a few selected air emissions which are commonly reported and used as key performance indicators; for a full inventory of air emissions, please refer to the complete LCI table in the annex of this report. The negative values for the biogenic carbon dioxide emissions are caused by the plant growth of the bio-based resources.

[2] Cooling water can be processed (softened), deionised, tap, ground, river or sea water, dependent on the location, applied technology and necessary temperature level and site specific frame conditions. Data for differentiation of water amounts used for cooling and processing due to lack of specific meters only partly available2

Table 10: Selected air emissions per 1 kg APP

Air emissions	kg
Carbon dioxide, fossil (CO_2, fossil)	1.73
Carbon dioxide, biogenic (CO_2 biogenic)	- 0.12
Carbon monoxide (CO)	1.15E-03
Methane (CH_4)	6.60E-03
Sulphur dioxide (SO_2)	2.97E-03
Nitrogen oxides (NO_x)	3.22E-03
Particulate matter ≤ 10 µm (PM 10)	1.87E-04

Wastewater Emissions

Table 11 shows a few selected wastewater emissions which are commonly reported and used as key performance indicators; for a full inventory of wastewater emissions, please refer to the complete LCI table in the annex of this report.

Table 11: Selected water emissions per 1 kg APP

Water emissions	kg
Biological oxygen demand after 5 days (BOD 5)	3.30E-05
Chemical oxygen demand (COD)	9.17E-04
Total organic carbon (TOC)	5.62E-05

Solid Waste

Table 12 below lists the solid wastes at unit process level before treatment.

Table 12: Solid waste generation per 1 kg APP (key foreground process level)

Waste for –	Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Non-hazardous	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hazardous	1.35E-03	0.00E+00	1.85E-03	0.00E+00	3.20E-03
Unspecified	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Total	1.35E-03	0.00E+00	1.85E-03	0.00E+00	3.20E-03

The End-of-life scenarios for different waste fractions is considered in partial stream calculations; i.e. the resource depletion and emissions referring to incineration and landfilling and the respective credits for energy gain depend on calorific value and actual elementary composition, which is relevant for the life cycle assessment. This is independent from the official attribution into hazardous/non-hazardous categories not consistently provided in the data collection.

Life Cycle Impact Assessment

The results for the impact assessment are calculated applying characterisation factors according CML 2001, update April 2013.

Input

Natural Resources

Table 13: Abiotic Depletion Potential per 1 kg APP

Natural resources	Value
Abiotic Depletion Potential (ADP), elements [kg Sb eq]	1.05E-06
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	59.46

Output

Climate Change

Table 14: Global Warming Potential (100 years) per 1 kg APP

Climate change	kg CO_2 eq.
Global Warming Potential (GWP), incl. biogenic carbon	1.82
Global Warming Potential (GWP), excl. biogenic carbon	1.95

Acidification

Table 15: Acidification Potential per 1 kg APP

Acidification of soils and water bodies	g SO_2 eq.
Acidification Potential (AP)	5.59

Eutrophication

Table 16: Eutrophication Potential per 1 kg APP

Eutrophication of soils and water bodies	g PO_4^{3-} eq.
Eutrophication Potential (EP), total	1.10

Ozone Depletion

Table 17: Ozone Depletion Potential per 1 kg APP

	g CFC-11 eq.
Ozone Depletion Potential (ODP)	2.22E-07

Summer Smog

Table 18: Photochemical Ozone Creation Potential per 1 kg APP

	g Ethene eq.
Photochemical Ozone Creation Potential	2.04

Dust & Particulate Matter

Table 19: PM10 emissions per 1 kg APP

Particulate matter	**g PM10 eq.**
Particulate matter ≤ 2.5 µm	9.02E-02
Particulate matter 2.5-10 µm	9.70E-02
Particulate matter PM10	**1.87E-01**
Particulate matter > 10 µm	6.18E-02
Total particulate matter	**2.49E-01**

Dominance Analysis

Table 20 shows the main contributions to the results presented above. A weighted average of the participating producers is used. In all analysed environmental impact categories, the precursors contribute to more than 80% of the overall impact (except for EP).The grouping “Precursors and Process” cover the environmental burden of the supply chain for terephthalic anhydride and polyol. The direct emissions of the polymerisation step not covered in one of the other groups (mainly NMVOC and water vapour) are also included here, but their contribution to any of the impact categories can be neglected (< 1%). The group “Other chemicals” covers additives, which also show relevant influence to the categories AP, ADP elements and EP (major relevance).

Electrical and thermal energy of the considered foreground production process contributes mostly to GWP. Whereas the waste treatment does not show any relevant contribution, the transport has notable environmental impact regarding the AP and EP indicators.

Table 20: Dominance analysis of impacts per 1 kg APP

	Total Primary Energy [MJ]	ADP Ele-ments [kg Sb eq.]	ADP Fossil [MJ]	GWP [kg CO_2 eq.]	AP [g SO_2 eq.]	EP [g PO_4^{3-} eq]	ODP [g CFC-11 eq]	POCP [g Eth-ene eq.]
Precursors and Process[1)]	90.39%	85.17%	93.03%	91.45%	80.83%	39.84%	94.02%	97.08%
Other chemicals	4.92%	11.16%	2.67%	-1.92%	8.42%	52.61%	1.27%	2.23%
Utilities[2)]	0.10%	1.53%	0.07%	0.18%	0.21%	0.11%	0.57%	0.05%
Electricity	1.69%	1.14%	1.16%	3.38%	2.22%	1.30%	3.93%	0.45%
Thermal Energy	2.30%	0.77%	2.43%	4.85%	1.11%	0.88%	0.10%	0.58%
Transport	0.60%	0.10%	0.64%	1.57%	7.09%	4.79%	0.08%	-0.40%
Process waste treatment	0.00%	0.13%	0.00%	0.47%	0.12%	0.47%	0.03%	0.02%
Total	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%	100.00%

[1)] Process = direct process emissions
[2)] Including water, catalyst, nitrogen, compressed air

Comparison of the Present Eco-profile with its Previous Version (2010)

Table 21 compares the present results with the previous version of the Eco-profiles of APP without flame retardant.

Table 21: Comparison of the present Eco-profile of APP with its previous version (2010)

Environmental Impact Categories	Eco-profile APP (2010)	Eco-profile APP (2015)	Difference
Gross primary energy from resources [MJ]	74.15	70.06	-5.5%
Abiotic Depletion Potential (ADP), elements [kg Sb eq.]	- *	1.05E-06	-
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	-	59.46	-
Global Warming Potential (GWP) [kg CO_2 eq.]	2.58	1.82	-29.46%
Acidification Potential (AP) [g SO_2 eq.]	5.79	5.59	-3.4%
Eutrophication Potential (EP) [g PO_4^{3-} eq.]	1.02	1.10	+7.8%
Ozone Depletion Potential (ODP) [g CFC-11 eq.]	8.91E-05	2.22E-07	-99.9%
Photochemical Ozone Creation Potential [g Ethene eq.]	1.93	2.04	+5.7%

* the ADP impact published in the last Eco-profile was calculated using a different method, hence cannot be compared with the ones here.

Table 21 shows for most impact categories a reduction of the environmental impact of APP between the two versions, sometimes significant (in the case of GWP and ODP).

The dominance analysis above shows that both precursors' data and the energy data are significant for the Eco-profiles. Therefore, improvements in the performance of relevant supply chain processes (quantitive and qualitative changes regarding the input mix of material and thermal energy towards resources with less climate-related impact) as well as reduction of the consumed energy are reflected here in the reduction of primary energy consumption, as well as of CO_2 emissions.

Moreover, the composition of the average APP product has changed since 2010, both due to small changes in composition (e.g. replacement of energy intense raw materials by a higher share of bio-based raw materials) of individual products together with a higher market share of less climate intense products. Those effects together with a continuously reduced carbon footprint of electricity consumption over the years is leading to the decrease of this environmental impact. However, due to the confidentiality of this information, no quantitative analysis can be published on the impact of these changes.

The reduction in greenhouse gases (GHG) emissions, usually proportional to the reduction in energy when mostly fossil fuels are used, is here greater (-29.5% GHG emissions vs. -5.5% primary energy consumption), for several reasons:

- First, there were big changes in the phthalic anhydride dataset used as a input in the model: the emissions data on the oxidation process used for its synthesis were updated and the pre-chain (pyrolysegas and xylene production) was modified to reflect the technological improvements (reduction of xylene/naphtha consumption, improvement of energy efficiency, change of the thermal energy mix from fuel oil to natural gas)
- Moreover, the greater use of bio-based precursors by all manufacturers accounts for decreased CO_2 emissions in a cradle-to-gate LCA like here because of CO_2 uptake by plants.
- Finally, the GHG emissions reduction are also partly due to the partial use of recycled materials as precursors.

In the case of acidification potential, the reduction by 3.4% is due to reduced direct emissions, as well as emissions all along the process chain. It is in a similar range as the energy reduction and therefore reflects the increased technological improvements leading to better efficiency.

A 5.7% impact increase in POCP indicator is observed, due to the change of composition of the average APP product with regards to a component showing high POCP impact.

Regarding eutrophication potential, a slight increase (due to the increased share of bio-based raw materials) also is observed, but given the +/- 5% uncertainty common in LCA, it cannot be interpreted with certainty.

Finally, regarding ODP, the change is due to a change in GaBi energy datasets and characterization factors.

Reviews

Internal Independent Quality Assurance Statement

As part of the overall quality assurance during the preparation of this Eco-profile, thinkstep AG conducted an internal review of this work.

Internal Independent Quality Assurance Statement

On behalf of thinkstep AG and its subsidiaries

Document prepared by	Victoire Goust
Title	Project Manager
Signature	
Date	14.12.2015
Quality assurance by	Anja Lehmann
Title	Senior Consultant
Signature	
Date	14.12.2015
Approved by	Hannes Partl
Title	Regional Director Central Europe, Service
Signature	
Date	21.12.2015

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External Independent Review Summary

The subject of this critical review is the development of the Eco-profile for Aromatic Polyester Polyols (APP). Due to the fact that various APP products exist based on various precursor materials and respective production technologies, detailed discussions were held on whether it is possible to provide Eco-profile data for different types of APP products. However, out of the reasons as explained on page 14 of this report, only one aggregated dataset for one average APP product is presented.

The review process included various meetings/web-conferences both during the goal & scope definition phase at the beginning of this project and at the end based on the final results and report between the industry participants, the LCA practitioners and the reviewer. In particular, two web-conferences were held between the LCA practitioner and the reviewer, which encompassed a model and database review and spot checks of data and calculations. In these meetings, special attention was laid on the differences between the results of the study from 2010 and the results presented in this report. Furthermore, the final Eco-profile report was reviewed by the reviewer as well as industry participants involved in this project. 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 processes comprising the production of different types of APP and taking into account the specific production processes of the participating companies. Background data representing the main precursors as well as all other material and energy inputs were taken from the GaBi database. Primary industry data was collected from 5 producers of APP (5 plants in 4 different countries), which lead to an estimated overall representativeness of 75-85% of the installed EU27 production capacity in 2014.

The potential environmental impacts for APP are dominated by the precursors across all impact categories (except for EP). Besides, also electricity and thermal energy needed for APP production has an impact on the results with regards to GWP. For further details, please refer to the main report.

Due to the low number of participants and different types of APP with different raw material inputs and production technologies, the review usually requires an in-depth look into the data of the individual producers. However, due to confidentiality, this was only partially possible for the reviewer. Under the strict rule not to share any company-specific data or using anonymised data, a more detailed look into the underlying model, data and assumptions was carried out during the review meeting, however, a more transparent reporting is prohibitive due to the above mentioned confidentiality reasons.

As mentioned above, special attention was paid to the differences in environmental performance of this Eco-profile with the previous study from 2010 (in particular with regards to the indicator GWP). During the review meeting it was revealed that one main reason for the high reduction in GWP was the different datasets used for phthalic anhydride. This reason, together with the changed production shares amongst the participants, is responsible for the largest share of the differences. Again, for further explanations, please refer to the main report.

At the outset of this Eco-profile project possible approaches for partial disaggregation of APP Eco-profiles were discussed in detail. However, the industry participants uttered serious concerns with the partial disaggregation approach. The following reasons were given:

- Revealing the input materials (even if it is only based on the average APP product) already compromises confidentiality of company-specific data.
- The fact that the user of such a dataset can create an Eco-profile of an APP product that is unrealistic (e.g. due to the selection of background processes for specific input materials) and not representative of the current European market, is concerning to the APP manufacturers.

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 APP produced in Europe.

Name and affiliation of reviewer:

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

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2012-11

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