



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

# Benzene, Toluene, and Xylenes (Aromatics, BTX)

PlasticsEurope  
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# Environmental Product Declaration

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** (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. Further, they do not imply a value judgment between environmental criteria. This EPD describes the production of the polymer precursors benzene, toluene, and xylenes (BTX) from cradle to gate (i.e. from crude oil extraction to liquid BTX at plant). **Please keep in mind that comparisons cannot be made on the level of the precursors:** 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	PlasticsEurope & CEFIC/APPE
LCA Practitioner	IFEU – Institut für Energie- und Umweltforschung Heidelberg
Programme Owner	PlasticsEurope aisbl
Programme Manager, Reviewer	DEKRA Consulting GmbH
Number of plants included in data collection	50 steam cracker units; complemented by desktop study of subsequent steps.
Representativeness	Production in EU27 countries + Norway
Reference year	2010
Year of data collection and calculation	2007–2010
Expected temporal validity	2014
Cut-offs	None
Data Quality	Good
Allocation method	Mass allocation, except for: energy allocation for refinery

## Description of the Product and the Production Process

This Eco-profile and EPD represents the average industrial production of several petrochemical polymer precursors from cradle to gate.

### Production Process

Benzene, toluene, and xylenes are produced from three different feedstocks: (a) pyrolysis gasoline, a by-product of steam cracking of saturated hydrocarbons; (b) reformat, a product of catalytic reforming of naphtha; and (c) light oil, a condensate fraction of coke oven gas from coal pyrolysis. While benzene is predominantly (61 %) produced from pyrolysis gasoline, toluene and xylenes are mostly produced from reformat (70 and 86 %, respectively). This results in quite different environmental indicators. The model for this Eco-profile comprises extraction and refinery of crude oil and natural gas; steam cracking of hydrocarbons into lower olefins; catalytic reforming of naphtha; and the extraction of BTX from pygas and reformat. Additionally, hydrodealkylation of toluene is used for on-purpose production of benzene.

### Data Sources and Allocation

The modelling of steam cracking, catalytic reforming, and petroleum refinery is based on confidential process and emission data from several sites. Recent data for energy consumption, feedstock mix and CO<sub>2</sub> emissions have been provided by APPE for the majority of European steam crackers. Representative literature data have been used for the modelling of the extraction and production of BTX from pygas and reformat. The processes for BTX extraction and production have been allocated by mass; the petroleum refinery has been allocated by energy.

### Use Phase and End-of-Life Management

Disposal of waste from production processes is considered within the system boundaries this Eco-profile. The use phase and end-of-life processes of the polymer precursors are outside the system boundaries of this cradle-to-gate system.

## Environmental Performance

The tables below show the environmental performance indicators associated with the production of 1 kg of each respective polymer precursor. Please see the Eco-profile report for explanations.

### Input Parameters

Indicator	Unit	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Non-renewable energy resources <sup>1)</sup>						
• Fuel energy	MJ	29.1	16.1	18.3	18.6	8.1
• Feedstock energy	MJ	50.8	49.5	49.2	49.2	49.2
Renewable energy resources (biomass) <sup>1)</sup>						
• Fuel energy	MJ	0.3	0.2	0.2	0.2	0.1
• Feedstock energy	MJ	0.0	0.0	0.0	0.0	0.0
Abiotic Depletion Potential						
• Elements	kg Sb eq	4.6 x 10 <sup>-8</sup>	3.8 x 10 <sup>-8</sup>	3.5 x 10 <sup>-8</sup>	3.6 x 10 <sup>-8</sup>	2.7 x 10 <sup>-8</sup>
• Fossil fuels	MJ	74.1	61.0	62.8	63.1	53.5
Renewable materials (biomass)	kg					
Water use	kg	33.0	31.3	23.5	23.9	13.3
• for process	kg	3.1	2.6	2.5	2.5	1.8
• for cooling	kg	26.7	25.9	18.2	18.5	9.0

<sup>1)</sup> Calculated as upper heating value (UHV)

### Output Parameters

Indicator	Unit	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
GWP	kg CO <sub>2</sub> eq	1.86	1.22	1.43	1.45	0.79
ODP	g CFC-11 eq	5.2 x 10 <sup>-4</sup>	4.1 x 10 <sup>-4</sup>	5.6 x 10 <sup>-4</sup>	5.7 x 10 <sup>-4</sup>	2.7 x 10 <sup>-4</sup>
AP	g SO <sub>2</sub> eq	6.12	4.75	5.70	5.80	3.23
POCP	g Ethene eq	0.40	0.28	0.29	0.29	0.18
EP, terrestrial	g PO <sub>4</sub> eq	0.42	0.33	0.37	0.38	0.25
EP, aquatic	g PO <sub>4</sub> eq	0.84	0.73	0.77	0.77	0.66
Dust/particulate matter <sup>2)</sup>	g PM10	0.27	0.24	0.24	0.25	0.18
Total particulate matter <sup>2)</sup>	g PM10 eq	5.12	4.01	4.69	4.77	2.87
Waste	kg	4.3 x 10 <sup>-5</sup>	4.9 x 10 <sup>-5</sup>	5.7 x 10 <sup>-5</sup>	5.7 x 10 <sup>-5</sup>	5.1 x 10 <sup>-5</sup>

<sup>2)</sup> Including secondary PM10

### Additional Environmental and Health Information

Benzene has been classified as a human carcinogen by the International Agency for Research on Cancer (IARC). Not a consumer product in itself, it is used within the chemical industry to produce other chemicals. All handling of benzene must meet strict international standards to protect human health. Applied standards in industry are generally more stringent than required by regulations.

### Additional Technical Information

BTX are single-ring aromatic compounds. They are colourless, flammable liquids at room temperature. The largest fraction of benzene is converted to

ethylbenzene, cumene, and cyclohexane, which are precursors for polystyrene, polycarbonates, epoxy resins, and polyamides, respectively; toluene is converted to toluene diisocyanate, a precursor for polyurethane foams; p-xylene is converted to terephthalic acid and dimethyl terephthalate, i.e. monomers for PET production; o-xylene is converted to phthalic anhydride, a precursor for phthalate plasticisers.

### Additional Economic Information

BTX are used as starting materials for a wide range of consumer products: clothing, pharmaceuticals, cosmetics, computers, paints, vehicle components, sports equipment, and many others.

## Information

### Data Owner

**PlasticsEurope**

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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 2012-005, valid until 31 December 2015 (date of next revalidation review).

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

# 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 and their precursors 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 feedstock 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 or polymer precursors 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 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 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. For example

- benzene is converted to ethylbenzene, cumene, and cyclohexane, which serve as precursors for polystyrene, polycarbonates and epoxy resins, and nylon, respectively;
- toluene is further processed to toluene diisocyanate, a precursor for polyurethane foams;
- p-xylene is mostly converted to terephthalic acid and dimethyl terephthalate, both monomers for PET production;
- o-xylene is used for the production of phthalic anhydride, a precursor for plasticisers.

### Functional Unit and Declared Unit

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

*1 kg of polymer precursor (here BTX aromatics) »at gate« (production site output) representing a European industry production average.*

## Product and Producer Description

### Product Description

Benzene, toluene and xylenes (*ortho*-, *para*-, and mixed xylenes) are single-ring aromatic compounds. Their chemical structure is shown in Figure 1 and their physical data is shown in Table 1. All of them are colourless, flammable liquids at room temperature. They are mostly used for the production of polymers and resins, and as motor fuel components.

### The commercial production of BTX aromatics

BTX aromatics are commercially produced based on three different feedstocks:

- Pyrolysis gasoline, a side product of thermal cracking (steam cracking) of hydrocarbons (e.g. naphtha, gas oil, ethane, propane, butanes)
- Reformate, a product of catalytic reforming of naphtha
- Light Oil, a condensate fraction of coke oven gas from coal pyrolysis

Additionally, the three aromatics can be chemically transferred into each other by means of transalkylation and disproportionation reactions (for example toluene to benzene and xylenes).

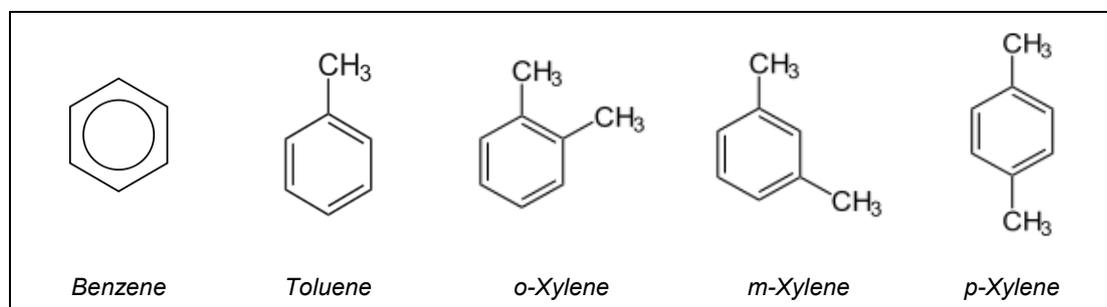


Figure 1: The chemical structures of BTX aromatics

Table 1: Characteristics and physical data of the polymer precursors under consideration in this Eco-profile

Name	IUPAC Name	CAS number	Molar Mass g/mol	Boiling Point °C	Gross Calorific Value MJ/kg
Benzene	Benzene	71-43-2	78.11	80.1	41.8
Toluene	Methylbenzene	108-88-3	92.13	110.6	42.4
o-Xylene	1,2-Dimethylbenzene	95-47-6	106.16	144.4	42.9
p-Xylene	1,4-Dimethylbenzene	106-42-3	106.16	138.4	42.9
Mixed Xylenes containing		1330-20-7	106.16	137-140	42.9
- o-Xylene (25%)	1,2-Dimethylbenzene	95-47-6	106.16	144.4	42.9
- m-Xylene (40%)	1,3-Dimethylbenzene	108-38-3	106.16	139.1	42.9
- p-Xylene (18%)	1,4-Dimethylbenzene	106-42-3	106.16	138.4	42.9
- Ethylbenzene (17%)	Ethylbenzene	100-41-4	106.16	136.15	43.0

Table 2: Production routes for BTX aromatics in 2012 (in wt.%) [APPE 2012]

Feedstock	Benzene	Toluene	Xylenes	Total BTX
Pyrolysis Gasoline	61 %	30 %	14 %	45 %
Reformate	26 %	70 %	86 %	47 %
HDA of Toluene	5 %	-24 % <sup>1)</sup>		3 %
Coking and HDA of others	8 %			5 %

<sup>1)</sup> Percentage of primary toluene used in hydrodealkylation (HDA)

In Europe (EU27) aromatics are mainly produced via pyrolysis gasoline and reformate.

Table 2 gives an overview of the shares of BTX aromatics produced by different routes. The mathematical model was built according to these shares. Since in Europe only 5 % of the BTX aromatics are produced from coke oven gas, this production route is not considered in this Eco-profile.

Raw pyrolysis gasoline has to be **hydrotreated** to saturate mono- and diolefins (to prevent polymerisation) and to remove sulphur compounds. This is usually done in two stages. In the first stage, a mild selective hydrotreating converts acetylenes, dienes, and styrene to olefinic compounds. In the second stage, olefins are saturated and residual sulphur is removed at higher temperatures (around 300 °C). For hydrotreatment, hydrogen from refinery processes is usually used. The further processing steps of hydrotreated pyrolysis gasoline and reformate are basically identical. A process scheme is shown in Figure 2.

The feedstock (either hydrotreated pyrolysis gasoline or reformate) is **fractionated** in a first distillation column into a benzene/toluene cut, which contains also 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. Both low temperature (20–40 °C) and high temperature (100–200 °C) processes at atmospheric pressure are common.

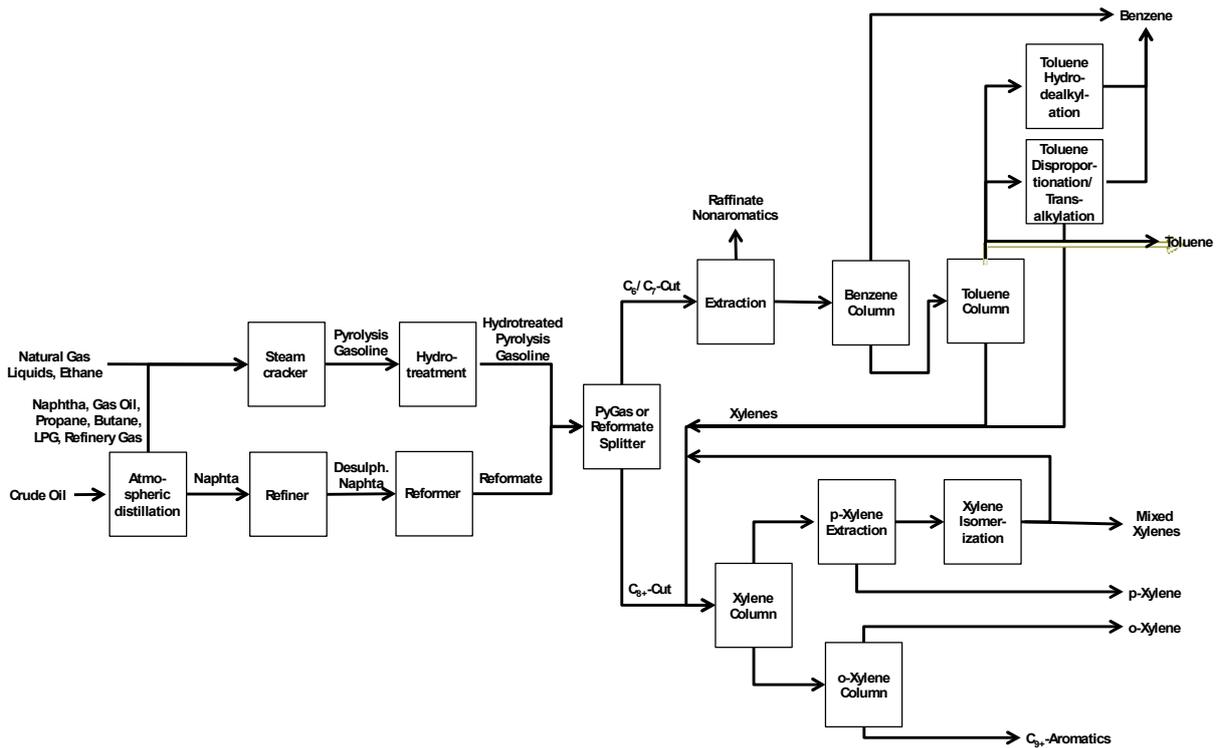
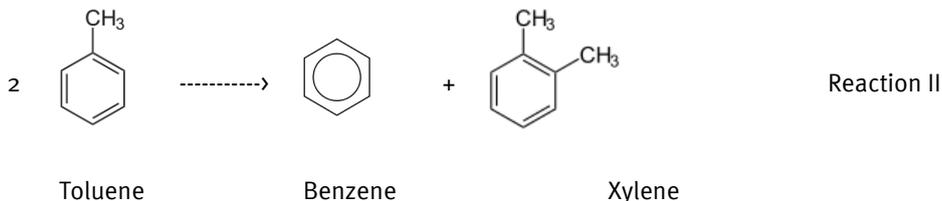
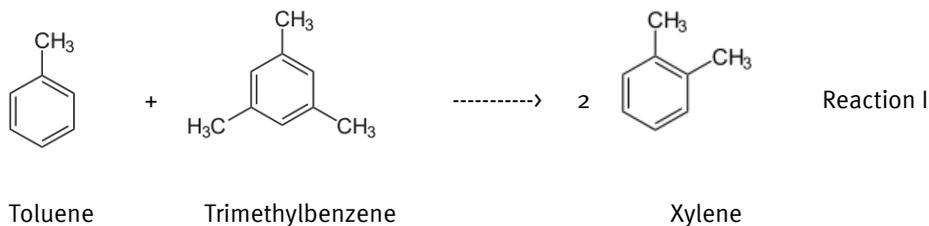
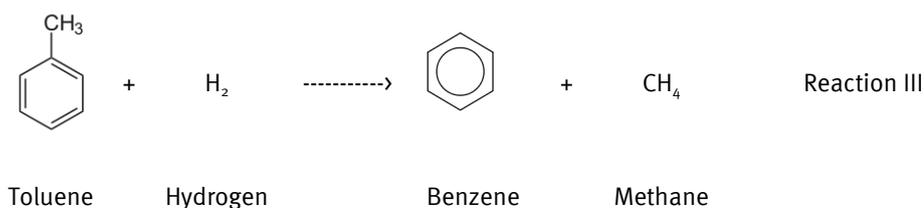


Figure 2: Process scheme for the production of benzene, toluene, and xylenes in a petrochemical complex

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 (Reaction I). During disproportionation, two toluene molecules react to form one molecule of benzene and xylenes, respectively (Reaction II). 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 (Reaction III). 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 recover also a part of o-xylene in the bottoms. In the latter case, o-xylene can be obtained as product after another distillation step. Higher aromatics ( $C_{9+}$ ) 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. After separation from light by-products (light ends (methane and hydrogen), benzene, toluene) through fractionation and from unsaturated components by clay treating the mixed xylenes (and by-product  $C_{9+}$ -aromatics) are recycled to the xylene column. The usual operating conditions are situated in the range of temperatures between 400–500 °C, pressures of 10–20 bar, and molar ratios  $H_2$ /feed of 15–20.

### Upstream Processes

To achieve appropriate LCI results in this study, especially concerning air emissions, the upstream processes are of high importance. The burdens of these processes (e.g. energy demand and emissions) are transferred to their products according to the allocation rules discussed on pages 24f. In the following sections, the relevant upstream processes are described in more detail. Included are:

- Upstream chains of crude oil, natural gas, natural gas liquids and refinery gas;
- Petroleum refinery processes including the catalytic reforming of naphtha;
- Steam cracking: for more details on the process of steam cracking and on refinery processes please refer to the PlasticsEurope Eco-profile of Ethylene, Propylene, Butadiene, Pyrolysis Gasoline, Ethlene Oxide (EO), Ethylene Glycols (MEG, DEG, TEG) [PLASTICSEUROPE 2012].

### Upstream chains of crude oil and natural gas

To illustrate the relevance of an up-to-date upstream chain, some characteristics of the pre-chains of crude oil and natural gas are shown in Table 3 and Table 4. For the compilation of this Eco-profile, using up-to-date data of the steam crackers upstream chains was a key issue. 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 NGL and ethane from North Sea fields were derived subsequently. Unconventional 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.

Table 3: Key figures for the upstream chain of crude oil according to provenance

Countries of origin	Share [wt.-%]	Crude oil in ground req'd per kg crude oil at refinery [kg]	Efficiency [%]	CO2 emission per kg crude oil at refinery [kg]
Libya, Algeria, Angola	11.1%	1.0282	97.26	0.2890
Middle East, Azerbaijan, Kazakhstan	22.9%	1.0491	95.32	0.2906
Netherlands	0.3%	1.0018	99.82	0.0304
Nigeria	4.3%	1.0123	98.78	0.4468
Norway, Denmark	15.7%	1.0038	99.63	0.0692
Russia	32.8%	1.0333	96.78	0.2014
United Kingdom	10.1%	1.0082	99.19	0.1980
Venezuela	2.8%	1.0947	91.35	0.4580
<b>Average EU27</b>		<b>1.0299</b>	<b>97.13</b>	<b>0.2278</b>

Table 4: Key figures for the upstream chain of natural gas according to provenance

Countries of origin	Share [vol.-%]	Natural gas in ground req'd per kg gas feedstock [kg]	Efficiency [%]	CO2 emission per kg natural gas feedstock [kg]
Algeria, Qatar	16.5%	1.1307	88.44	0.2888
Germany	6.4%	1.0513	95.12	0.1462
Netherlands	23.2%	1.0126	98.76	0.0274
Norway	23.6%	1.0337	96.74	0.0779
Russia	22.7%	1.1708	85.41	0.3487
United Kingdom	7.6%	1.0598	94.36	0.1533
<b>Average EU27</b>		<b>1.0791</b>	<b>92.98</b>	<b>0.1727</b>

## Petroleum refinery

Petroleum refineries are complex plants in which the combination and sequence of processes are usually very specific to the characteristics of the raw materials, i.e. the composition of the crude oil, and the products to be produced. Refineries are not only different regarding their configuration, process integration, feedstock, product mix, unit size design and control systems. Differences in market situation, location and age of the refinery environmental regulation are amongst other reasons for a wide variety of refinery concepts.

**Model Development for European Refineries:** As the cracker feedstock and its pre-processing significantly influence the LCI results of the polymer precursors under consideration in this Eco-profile, the adequate modelling of the petroleum refinery as part of the upstream chain is a key issue for this Eco-profile of polymer precursors. In spite of the large variety of possible and actual refinery configurations, the Draft Reference Document on Best Available Techniques for Mineral Oil and Gas Refineries [BREF 2012] describes in its Annex II four typical refinery configurations – from a simple hydroskimming unit up to a complex refinery with hydroconversion and a hydrocracker and/or an Integrated Gasification Combined Cycle Unit (IGCC). The refinery model used for the calculation of the current Eco-profile is a model that represents all typical processes of the different refinery configurations. It considers the capacity weighted mixture of refinery configurations in Europe according to BREF 2012 and EUROSTAT 2011, taking the changed product mix in recent years in account. This detailed model comprises the single processes of a petroleum refinery and makes up an average model of the European refinery (see Figure 3).

As BREF 2012 does not only contain aggregated numbers or weighted averages of emission and energy/water consumption data, but also primary data of the majority of refineries in Europe in anonymous form, the data quality for this model is very good. This data has been complemented by various specific confidential refinery data, by numbers from Eurostat, e.g. for the mix of energy sources for process energy, and by literature data from widely acknowledged sources such as MEYERS 2003 and others. In the cases BREF 2012 mentioned a range of values for process parameters the arithmetic averages were applied. After adopting the model to the up-to-date mass and energy flows within European refineries, it has been validated by comparing its results to the data of BREF 2012, Eurostat and EPER.

**Process Technology** [BREF 2012, ULLMANN 2010]: The process within the refinery that is of high relevance for the subsequent steam cracking is the atmospheric distillation of crude oil. Most other energy and emission intensive processes of a refinery are more relevant for products, which are usually not used as a steam cracker feedstock. Therefore, only the processes for pre-treatment of crude oil feedstock and atmospheric distillation are described in detail. Furthermore, the process of catalytic reforming of naphtha is described, since reformat gasoline, one of its products, is used as a feedstock to the aromatic extraction and production plant.

**Desalting:** Crude oil and heavy residues contain varying quantities of inorganic compounds such as water, soluble salts, sand, silt, rust, and other solids, together characterized as bottoms sediment. Those impurities, especially salts could lead to fouling and corrosion of heat exchangers and especially the crude distillation unit overhead system. Therefore desalting of the incoming crude is generally applied before separating it into fractions. The principle of desalting is to wash the crude oil or heavy residues with water at high temperature and pressure to dissolve, separate and remove the salts and solids. After preheating to 115–150 °C, the oil feedstock is mixed with water in order to dissolve and wash out the salts. The water must then be separated from the oil feedstock in a separating vessel by applying a high potential electric field across the settling vessel to coalesce the polar salt water droplets or by adding demulsifier chemicals to assist in breaking up the emulsion. Many refineries have more than one desalter.

**Atmospheric Distillation:** The next step – and the most important one regarding cracker feedstock – is atmospheric distillation, which is the first and fundamental separation process in a refinery. In the atmospheric distillation unit, crude oil is heated to temperatures of 300–400 °C and then subjected to distillation under atmospheric pressure separating the various fractions according to their boiling range. Heavier fractions from the bottom of the atmospheric distillation unit can be further separated by subsequent vacuum distillation. The products from the crude distillation unit, ranging from the lightest to the heaviest cut, are: naphtha and light components (boiling < 180 °C), kerosene (boiling range: 180–240 °C), light gasoil (240–300 °C), heavy gasoil (300–360 °C) and atmospheric residue (boiling > 360 °C). These fractions are separated by condensing on 30–50 fractionation trays. The lighter fractions condense and are collected towards the top of the vertical distillation column. The overhead of this column is the light fraction, non-condensable refinery fuel gas. Most of the fractions resulting from atmospheric distillation can be sold directly for use in the petrochemical industry (the route which naphtha and atmospheric gas oil take), as finished products after hydrotreatment, or be blended with products from downstream processes, e.g. heavy gas oil being mixed into diesel. So leaving the atmospheric distillation unit the straight-run unstabilised naphtha is passed to a naphtha splitter, separating the share for the petrochemical industry (industrial spirit), already in condition to be fed to the steam cracker, from the stream that is fed to the hydrotreater. During hydrotreatment, unsaturated light hydrocarbons in the straight-run naphtha are saturated and sulfur is removed by reaction with hydrogen. Saturated light hydrocarbons are separated from naphtha and either sold to the market or used as feedstock for the steam cracker (propane, butane or a propane/butane mix as liquefied petroleum gas). The third relevant feedstock for steam cracking from the petro-

leum refinery is atmospheric gas oil which can be taken directly from the atmospheric distillation unit and be used as a feed.

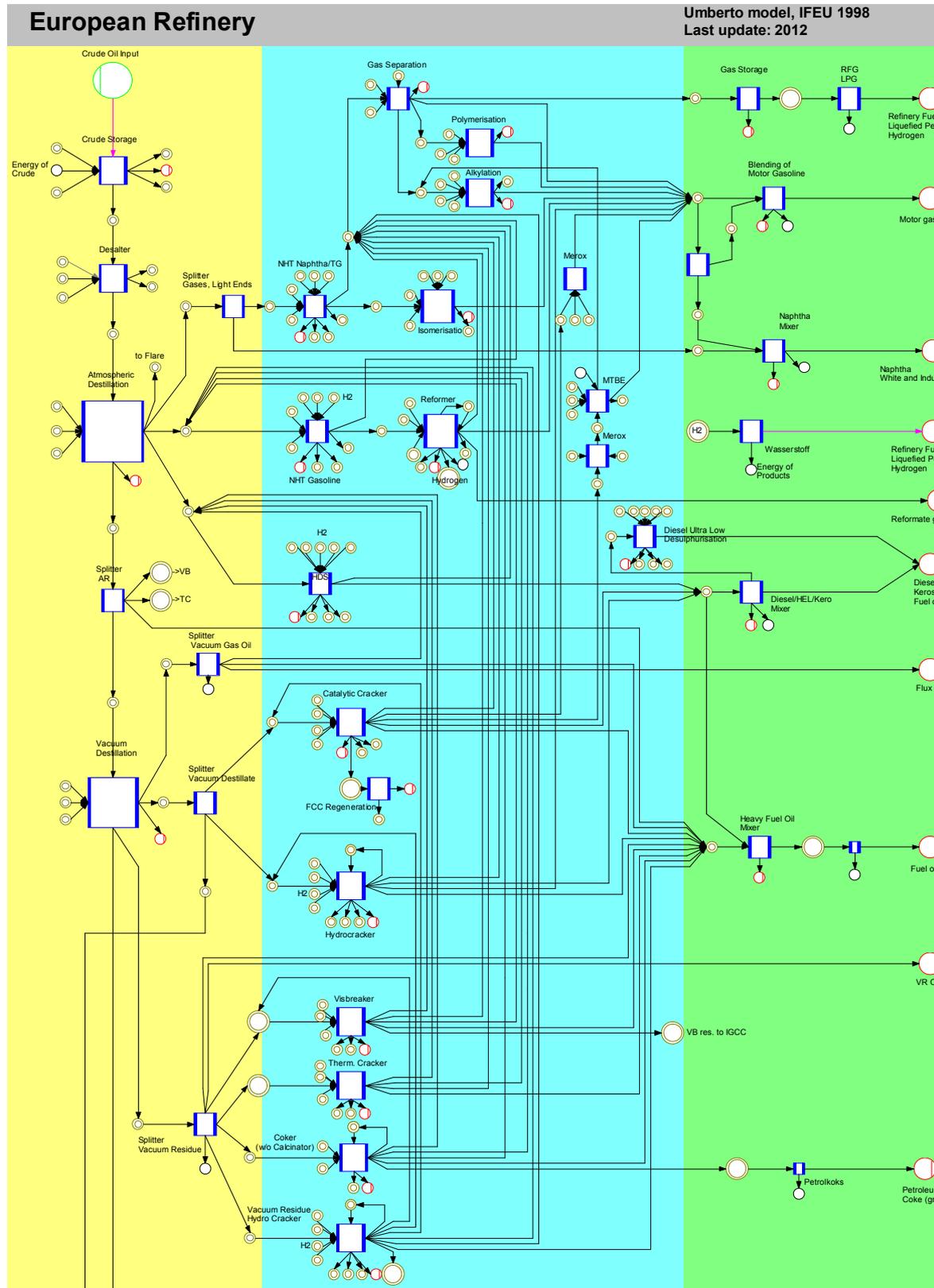


Figure 3: Petroleum refinery model in UMBERTO (Source: IFEU 2012)

**Catalytic Reforming:** The purpose of catalytic reforming is to improve the octane number of hydrocarbon mixtures by converting paraffins to iso-paraffins and naphthenes and the conversion of naphthenes to aromatic compounds. Typically straight-run or other low-octane naphtha is used as feedstock. A mixture of hydrotreated naphtha and hydrogen is first fed to a furnace, where the mixture is heated to the desired temperatures (450-520 °C), and then to several (up to five) fixed-bed catalytic reactors installed in series. Since the reactions are endothermic, reheaters are located between adjoining reactors. During operation the catalyst activity decreases due to the formation of coke deposits. The catalyst can be regenerated in an oxygen-rich atmosphere. To keep a stable production process, various methods are applied for regeneration, e.g. moving-bed technology or the installation of an additional swing-reactor, so that one reactor is always under regeneration. The product received from the last reactor is cooled and sent to a high pressure separator. The hydrogen-rich gas from the top of the separator is split into two streams. One stream is recycled while the other represents excess hydrogen, which is directed to the refinery hydrogen system for further use. The liquid bottom product from the separator is sent to a debutaniser, where butanes and lighter gases are separated from the higher boiling bottom product called reformate. The liquid reformate, containing up to 70 vol.-% aromatics, is either fed to the gasoline pool or used as feedstock in an aromatic extraction and production plant.

### Steam cracking as a process for the production of pyrolysis gasoline

Steam cracking is a process to split up longer, saturated hydrocarbons into shorter, unsaturated compounds under high temperature (700-875 °C) and in the presence of steam. The main products of steam cracking are ethylene, propylene, and methane, their shares depending on the feedstock. Important minor products are butadiene and, in case of naphtha or gas-oil feedstock, pyrolysis gasoline with high aromatic content. In the European Union crackers are basically fed with naphtha and condensates, also called natural gas liquids (NGL). Both sorts of feedstock are very similar mixtures of hydrocarbons. Naphtha is an important product of the oil refinery, with a boiling range in between 50 and 190 °C. Liquid feedstocks have a high share as they are transported easily. Other important feedstocks for crackers in the EU are gas oil, butane, propane, refinery gas, and ethane (see Table 5). Ethane mainly comes from North Sea gas fields whereas other feedstock gases come from refineries.

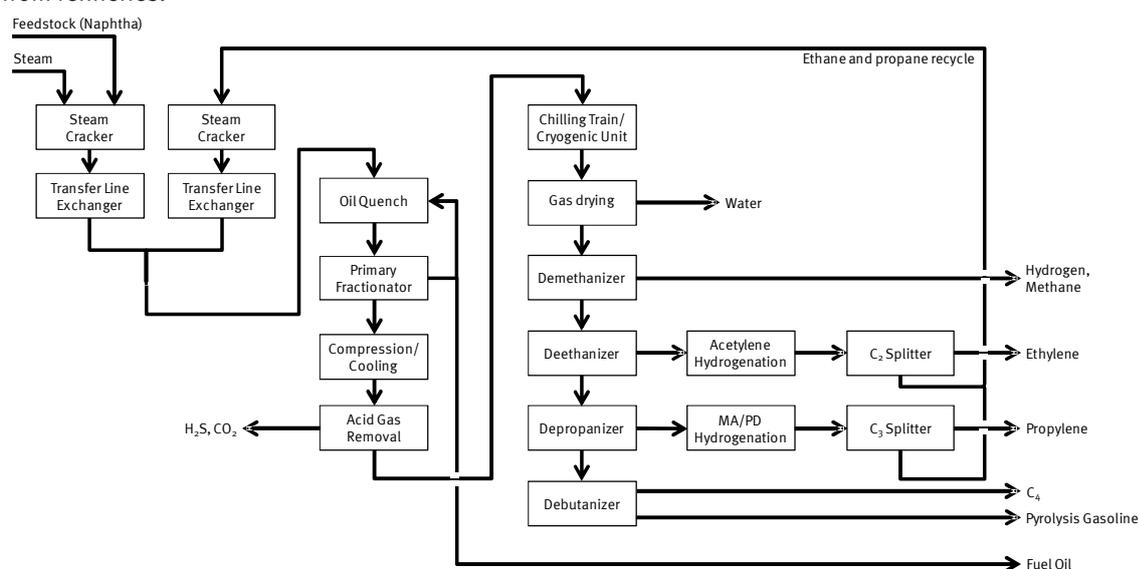


Figure 4: Schematic flow diagram showing the lower olefin production in a naphtha-based front-end demethanising steam cracker

Table 5: Feedstock for crackers in the European Union 2008-2010 [APPE 2012]

Feedstock	Share [%]
Ethane / Refinery gases	4 %
Propane / Butane / LPG	12 %
Naphtha / Condensates (NGL)	74 %
Gas oil	6 %
Others (incl. C4)	4 %

**Process Technology:** Only a limited number of international technology contractors license the equipment used for crackers. The generic design of the cracking units is quite similar. Little modifications help to optimize the plant performance according to local conditions. Besides differences in furnace design, pressure and temperature of the fractionation columns and refrigeration systems may vary or turbo expanders may be in use. Regardless of feedstock or contractor a cracker complex may be separated into three sections namely pyrolysis, primary fractionation/compression and product fractionation as shown in Figure 4.

In the **pyrolysis section (steam cracker)** the hydrocarbon feedstock is preheated and then vaporised with superheated steam before passing into long and narrow tubes arranged in a cracking furnace. In this reactor, the hydrocarbon feedstock is cracked into smaller molecules. The product distribution of the product can be controlled through variation of residence time, temperature profile, and partial pressure. This process is highly endothermic and therefore requires high energy input. Therefore the tubes of the furnace are heated to 750 – 875 °C by oil or gas fire burners. To reduce the partial pressure of the hydrocarbon mixture and to minimise coke formation high-pressure steam is injected which gives the process the name steam cracking. To quickly quench the product gases to 550 – 650°C and to recover heat for internal use, transfer line exchangers (TLEs) may be used.

The **primary fractionation and compression section** consists of the primary fractionator (naphtha and gas oil feed only), quench tower, gas compressor and gas clean-up facilities. The primary fractionator is used to condense and fractionate fuel oil streams produced from naphtha and gas oil fed crackers. The gases are de-superheated in the quench tower by a circulating oil or water stream. The circulating oil or water stream is used as a medium level heat source for the rest of the plant. Product gases from the quench tower are condensed by four or five stages of gas compression. The gas is cooled after each stage and passed through a liquid knock-out drum. Finally, acid gases and carbon dioxide are removed from the cracked gas.

In the **product fractionation section** products are cooled down and subsequently fractionated. The first chilling train usually consists of four or five successive stages of chilling, incorporating ethylene and propylene refrigeration as well as an elaborate self-refrigeration system. This produces hydrogen, which is used for downstream hydrogenation or hydrotreating of the heavier products or sold as a product. The exact process flow sequence varies according to the feedstock and the design arrangement, but various fractionation towers are used to separate the desired products. This may include a sequence of de-methaniser, followed by a de-ethaniser. Bottoms from the de-ethaniser are directed to the de-propaniser and the de-butaniser. The lighter the feedstock, the fewer fractions need to be separated and the separation system may be constructed less complex. After separation, the ethylene still contains undesirable acetylene and ethane. Acetylene is either converted to ethane and ethylene by selective catalytic hydrogenation or removed by extractive distillation. After separation of ethylene and ethane, ethane is recycled back to the cracker. Similarly the C<sub>3</sub> fraction contains methyl acetylene (=propine) and propadiene after separation. Selective hydrogenation is used to convert this into propylene and propane prior to separation in a C<sub>3</sub> splitter.

**Products and their further use:** Ethylene is an important precursor for the organic chemical industry and it has a wide range of derivatives. More than 50 % of ethylene is used in the production of polyethylene, but it is also very important for the production of polystyrene (via ethylbenzene and styrene), glycols, vinyl acetate and PVC. Propylene is mostly used to produce polypropylene (more than 50 %) but also for the production of acetonitrile, a precursor of acrylic esters, and propylene oxide. About half of butadiene is used to produce styrene/butadiene rubbers and latexes. A further quarter is used for polybutadiene rubber, most notably ethylene-propylene-diene monomer (EPDM) rubber. It is also used for the production of adiponitrile – a precursor for nylon production. From pyrolysis gasoline (pygas), benzene, toluene, and xylenes (BTX-aromatics) are extracted, all of them being used as precursors in the polymer industry.

### **Producer Description**

This Eco-profile represents European industry averages within the scope of PlasticsEurope as the issuing trade federation. Hence it is not attributed to any single producer, but rather to the European plastics industry and their suppliers in the petrochemicals sector, as represented by PlasticsEurope's and APPE's membership.

# Eco-profile – Life Cycle Inventory

## System Boundaries

This Eco-profile refers to the **production of polymer precursors** and is based on a **cradle-to-gate system** (Figure 5). 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 (e.g. by pipeline or ship). In this cradle-to-gate information module, the subsequent steps of polymer production, conversion, use phase and end-of-life management are not included.

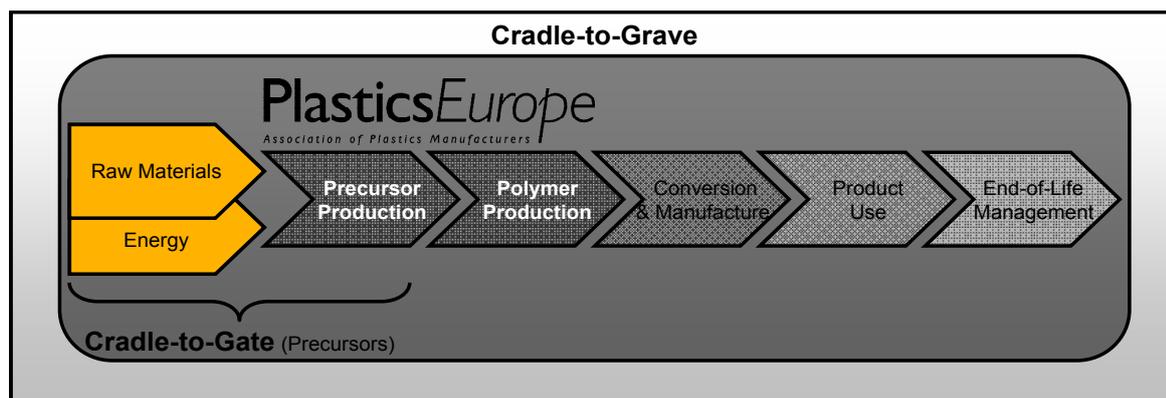


Figure 5: Cradle-to-gate system boundaries (Source: PlasticsEurope)

## Cradle-to-Gate System Boundaries for Production

The following processes are included in the cradle-to-gate LCI system boundaries (see also Figure 6):

- 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 is outside the LCI system boundaries. The end-of-life treatment of the polymer precursors and their resulting products is also outside the LCI system boundaries of this Eco-profile. Inputs and outputs of secondary materials and wastes for recovery or disposal are noted as crossing the system boundaries. An exception is low-radioactive waste from electricity generation for which a final storage has not been found yet; it is declared as output.

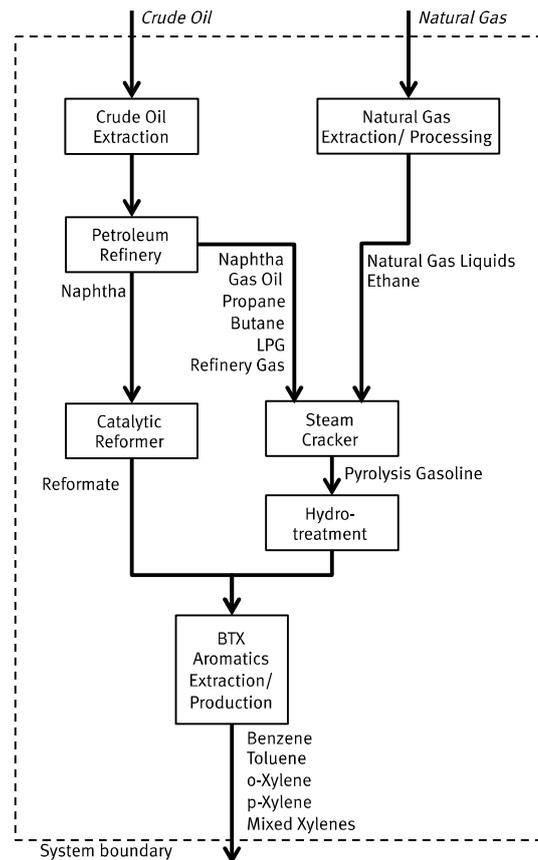


Figure 6: Schematic flow chart of the production processes for the polymer precursors under consideration (here BTX aromatics).

### Technological Reference

The LCI data in this Eco-profile represents the average applied technology for the production of polymer precursors in Europe as shown in Figure 6. It is based on confidential data by some producers as well as on representative literature data. As the production processes are not under control of PlasticsEurope's member companies primary data could not be obtained systematically. Thus the coverage as percentage of the total production volume cannot be stated. Nevertheless, the overall data of the aromatic complex and of the core upstream process of steam cracking was reviewed by APPE, the Association of Petrochemicals Producers in Europe, which represents the European petrochemical industry. Based on a survey of APPE for the European Emission Trading System (EU ETS) the Eco-profile model for steam cracking could be verified and amended with actual industry data from 2008 – 2010. Due to this fact the representativeness of the process data is estimated to be at least 80 % and the technological coverage for this Eco-profile is estimated to be at least 90 %.

Crackers using gas feedstock, such as ethane, propane or butane are hardly in use within the EU27. However, they are represented in the data set in the adequate proportion.

According to the PlasticsEurope LCI methodology [PLASTICSEUROPE 2011] Eco-profiles shall differentiate

- primary data from **foreground processes**, i.e. those that are under operational control, and
- secondary data from **background processes**, i.e. those operated by third parties where only indirect management control or no control exists.

Thus, all processes under consideration in the present Eco-profile are background processes according to the above-mentioned methodology as they are not under operational control of PlasticsEurope.

However, due to their relevance for the results of this Eco-profile (and subsequent Eco-profiles for polymers) all processes taking place within the system boundaries have been treated like foreground processes as far as research on and validation of the underlying data are concerned.

According to the PlasticsEurope LCI methodology and product category rules inputs of secondary materials (recyclate) and outputs of waste for recovery or disposal shall be noted as crossing the system boundaries. While there is no input of recyclates at all, outputs of wastes for recovery or disposal only contribute very little to the total proceedings under consideration in this Eco-profile.

### **Temporal Reference**

The LCI data for this Eco-profile represents the most recent available data and therefore represents the average technology in Europe. For the petroleum refinery the collected data is from the time period 2007-2010, mostly from 2009. The data for steam cracking is from the years 2008-2010. For BTX aromatics, production data of the year 2010 was used as basis for calculation whereas the literature data used for modelling of the unit processes originates from the years 1995-2003. This data is considered to be still valid since the production facilities have high investment costs and therefore the data underlies small changes only. For the upstream chains of the feed-stock most data was collected for the year 2009; a few exceptions of the data originate from the years 2007-2008.

The overall reference year for this Eco-profile is 2010 with a maximum temporal validity until 2014.

### **Geographical Reference**

This Eco-profile refers to the average production of polymers precursors in the EU27 member states (+Norway). The LCI data describing direct inputs and outputs of the production processes is representative of the defined production region. In order to be applied in other regions adjustments might be required.

### **Cut-off Rules**

To achieve completeness, i.e. a closed mass and energy balance, any cut-off of material and energy flows has been avoided in this Eco-profile. For commodities with an input < 1 % of the respective polymer precursor's output, e.g. NaOH and HCl, generic datasets from the LCA database Ecoinvent v2.2 [ECOINVENT 2010] have been used.

Simplified generic processes are assumed for catalysts and a few commodities (input < 0.1 % of the precursor's output) with missing secondary production data. The process input/output relation has been determined by reaction equations from literature. The upstream production of the used metals (antimony, cobalt, manganese and palladium) and chemicals are implemented using Ecoinvent v2.2 data. Thus, the potential environmental relevant metal extraction and refinement processes are included in the LCI data.

## **Data Quality Requirements**

### **Data Sources**

The LCI data used in this Eco-profile is representative of the production processes of polymer precursors in Europe, both in terms of technology and market share.

The modelling of the petroleum refinery is 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 2007 – 2009 [EUROSTAT 2011].

The modelling of the steam cracking processes [PLASTICSEUROPE 2012] is 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 CO<sub>2</sub> emissions for the majority of European plants [APPE 2012], which for reasons of confidentiality appears in form of an aggregated average in the final model.

The modelling of the processes for BTX aromatics extraction and production are 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 (Table 2), and specific process data.

The upstream chains for the relevant feedstock, i.e. crude oil, natural gas, natural gas liquids (NGL) and ethane from the North Sea are based on the database ecoinvent v2.2 [ECOINVENT 2010]. The regional provenance mix has been updated with statistical data from Eurostat for the year 2009. The upstream chain has been updated, notably in view of its inputs and outputs, with primary data from the following environmental/annual reports:

- BP North Sea Region Environmental Statement 2010 [BP 2010]
- ENI Annual Report 2011 [ENI 2012]
- Gazprom Environmental Report 2009 [GAZPROM 2009]
- Lukoil Sustainability Report Russian Federation 2007-2008 [LUKOIL 2008]
- NOGEPa Annual Report 2009 [NOGEPa 2009]
- OLF Environmental Report 2010 [OLF 2010]
- Shell U.K. Annual Environmental Statement for Upstream Operations 2010 [SHELL 2010]
- WEG Annual Report 2009 Facts & Figures [WEG 2009]

Besides data from these publications has been used for the update of the upstream chains:

- Greenhouse Gas Emissions from the Russian Natural Gas Export Pipeline [WUPI 2005]
- Environmental and Economic aspects of using LNG as a fuel for shipping in The Netherlands [TNO 2011]

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]

Data sources of on-site energy and utilities

- Steam and electricity:  
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 (2008)
- Industrial gases: oxygen and nitrogen according to ecoinvent v2.2 [ECOINVENT 2010] and IFEU internal database
- Process and cooling water: ecoinvent v2.2 [ECOINVENT 2010]

### **Relevance**

With regard to the goal and scope of this Eco-profile, the collected process data, i.e. data for steam cracking, the BTX production and refinery processes, are of high relevance as these are the essential processes for production of polymer precursors in Europe. The environmental contributions of each process to the overall LCI results are shown in Chapter 'Life Cycle Impact Assessment'.

### **Representativeness**

The data is collected or updated according to goal and scope of this Eco-profile. The used data reflect the current technology in Europe and the current upstream chains of feedstock relevant for production in EU27 member countries. As the model of the processes steam cracking and BTX extraction and production was reviewed by APPE, the representativeness of the process data is assumed to be at least 80 % and the technological coverage for this Eco-profile is assumed to be at least 90 %.

### **Consistency**

Relevant process and upstream chain data have been validated to comply with goal and scope of this Eco-profile. Thus an overall consistency of the applied data can be stated.

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 throughout the whole system. Although all parts of the model are defined as background systems according to the PlasticsEurope LCI methodology [PLASTICSEUROPE 2011], all parts of the model have been treated with the same thoroughness as if they were foreground systems.

### **Reliability**

In this Eco-profile process data originates from a hybrid model of confidential operator data, confidential data from the Association of Petrochemicals Producers in Europe (APPE) and publicly available literature data as described in the section 'data sources'. Data of the upstream chains of the feedstock are based on the LCI database Ecoinvent v2.2 [ECOINVENT 2010] and have been updated by data from primary and secondary sources as described in the section 'data sources'. As the confidential data from operators and the association APPE is con-

sidered to be reliable and as data from literature sources was cross-checked by the LCI practitioners, the overall data for this Eco-profile is considered to be reliable.

### **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. Thus, the data is considered as complete for all relevant flows.

### **Precision and Accuracy**

The assessment of data precision is generally a difficult topic for LCA practitioners. It is desirable to calculate a confidence range for the LCI (and LCIA) results. Technically this confidence interval of the results could be calculated with the help of Monte-Carlo simulation (in Umberto5). For this, standard deviations (or distribution functions) of every flow and every unit process would have to be known that are not available in reality due to insufficient independent data points. An alternative option to determine the uncertainty could be an estimation of the standard deviations basing on a pedigree matrix, as practised e.g. in ecoinvent v2.2 [ECOINVENT 2010]. The disadvantage of this method would be that incorrect estimates of relevant flows would lead to wrong confidence intervals and basic misinterpretations of results. Hence a quantitative uncertainty assessment cannot be provided. The overall qualitative assessment of data accuracy is as follows:

- There is a high accuracy of relevant material flows, especially of intermediate products within the production system
- There is good accuracy for energy flows and combustion related air emissions (CO<sub>2</sub>, SO<sub>2</sub>, NO<sub>x</sub>, CH<sub>4</sub>)
- There is satisfactory accuracy for other air emissions and emissions to water bodies

### **Reproducibility**

All data and information used are either documented in this report or they are available from the processes and process plans designed within the Umberto5.6 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 of the core processes steam cracking as well as extraction and production of BTX aromatics was reviewed by APPE, and based on a survey of APPE, the Eco-profile model for steam cracking could be verified and amended with industry data from 2008 – 2010. The production data from the other sources mentioned above has been cross-checked with literature data. This literature as the Reference Documents on Best Available Techniques, ecoinvent v2.2 [ECOINVENT 2010] and Ullmann's Encyclopedia are considered to contain highly representative data.

The upstream chains of the feedstock have been validated after their update by comparing the emissions with different references, i.e. Gemis 4.6, ecoinvent v2.2 [ECOINVENT 2010], internal reference from IFEU. The changes of

emissions along the upstream chains of the feedstock are in accordance with the respective primary data and well to explain. The consistency of the overall input data is thus confirmed.

### Life Cycle Model

The life cycle system is modelled in UMBERTO5, a standard software tool for LCA (see Figure 7). The associated database integrates ISO 14040/44 requirements. Data for production processes have been transferred to the model after a successful data validation.

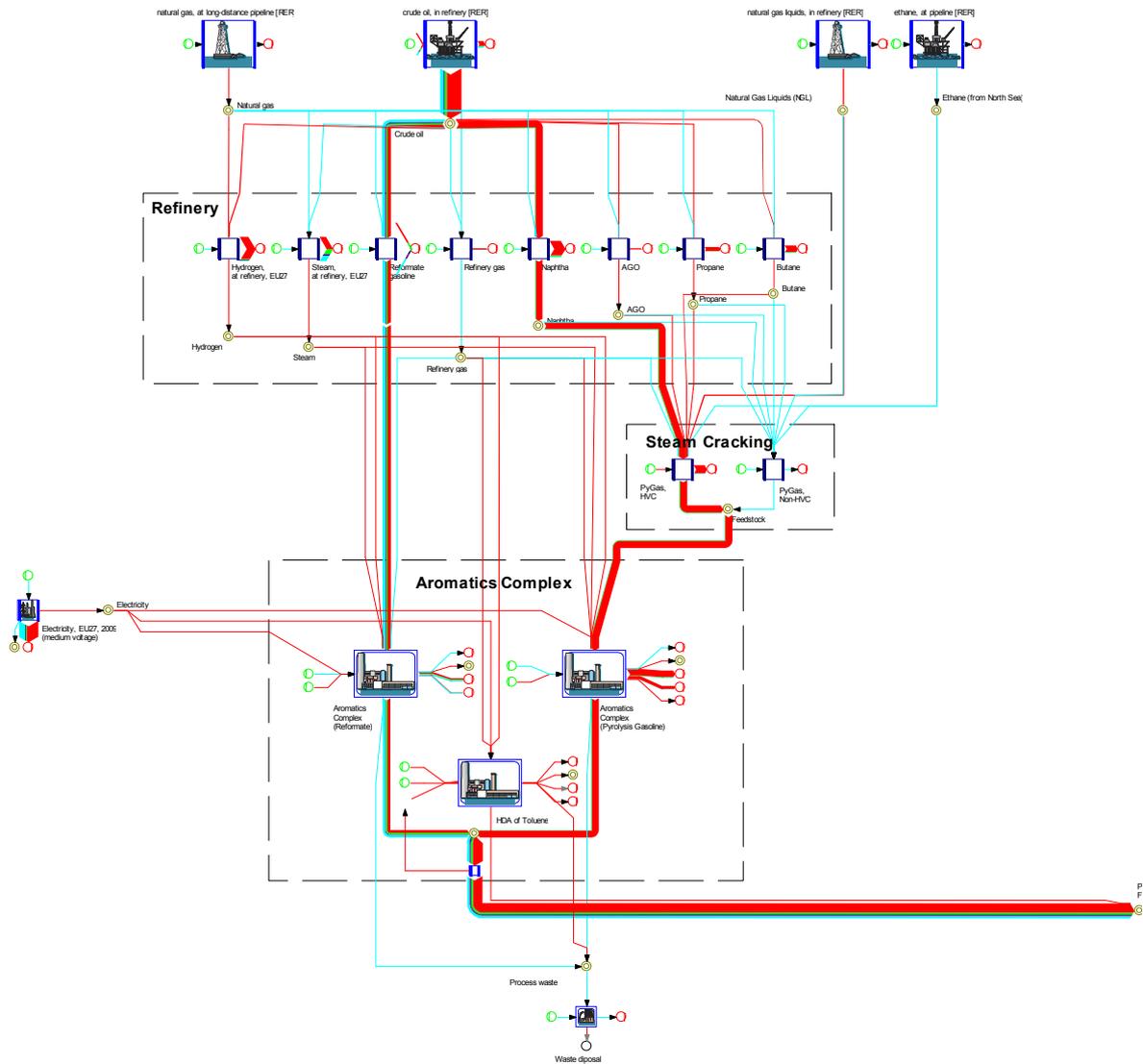


Figure 7: Life cycle model for the production of polymer precursors in Europe in UMBERTO5

Due to confidentiality reasons details on software modelling and methods used cannot be shown here. The calculation follows the horizontal calculation methodology, i.e. processes are aggregated each supplying the same reference flow.

### Calculation Rules

#### Vertical/Horizontal Averaging

According to the Plastics Europe methodology [PLASTICSEUROPE 2011], vertical averaging should be applied wherever possible to ensure relevance with regard to the supply chain situation. However, the petrochemical proc-

esses under investigation are outside the scope of PlasticsEurope as a federation and, in most cases, not under operational control of member companies. Hence, information on the supply chain of different aromatics producers or refineries was not available, and horizontal averaging, as shown in Figure 8, was applied instead. For the modelling and calculation of the Eco-profile at hand, European average models of the core processes were used. It is assumed that the averages are highly consistent anyway as the core process data for steam cracking and BTX aromatics production and extraction was verified with data from and by the Association of Petrochemicals Producers in Europe (APPE). The data for other processes in the upstream of the aromatics complex, i.e. petroleum refinery and pre-chains of the steam cracker's feedstock, are assumed to be highly consistent since the data was cross-checked with well-respected literature sources.

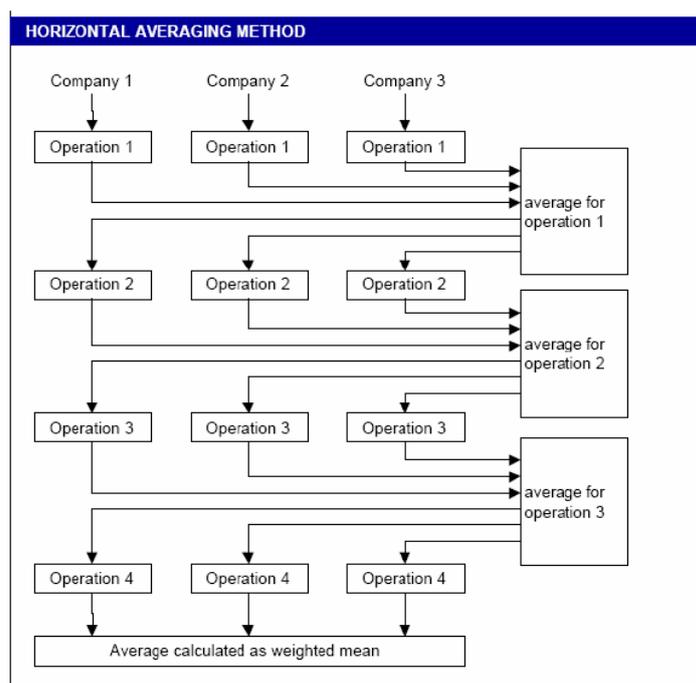


Figure 8: Horizontal Averaging (source: Eco-profile of high volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)

### Allocation Rules

Production processes in chemical and plastics industry are often multi-functional systems, i.e. they have not one, but several valuable product and co-product outputs. According to PlasticsEurope's LCI methodology and product category rules for uncompounded polymer resins and reactive polymer precursors v.2.0, 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.

In this Eco-profile, where the main production technologies for BTX aromatics are considered, avoiding allocation was not feasible since several processes with numerous products would have to be investigated. Moreover, the processes modeled here are the main source of BTX aromatics, making it difficult to identify a suitable process for implementing system expansion. 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.

Generally, physical allocation is applied in this Eco-profile. For the processes of BTX aromatics production, steam cracking, oil refining and the upstream chains of crude oil and natural gas the following allocation rules were applied:

- 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, auxiliaries, 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 other inputs and outputs (energy, auxiliaries, 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 ensure 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.

Economic allocation as an alternative suffers from uncertainties: the market prices for the considered products fluctuate greatly and some prices for intermediate products (e.g. of refineries) cannot be determined at all.

For steam cracking, another potential criterion for a physical allocation is the energy content of the products. This method leads to results similar to those of mass allocation, because the calorific values of the main products ethylene, propylene and butadiene are very similar. Also for the aromatics production and the petroleum refinery an alternative (mass, energy) based allocation method would not cause significant differences in the Eco-profiles. However, mass allocation for refinery processes would lead to higher burdens for heavy fractions and residues compared to low-boiling products, due to their higher density.

For end-of-life management, the allocation rule is: process waste with a recycling potential (e.g. catalysts) leaving the system (<0.5 wt.-%) 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](http://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) 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 values (lower heating value, LHV) are also presented in Table 6 for information purposes. For a discussion of the considerable differences between the products, please see section Comparison of the Present Eco-profile with its Previous Version.

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 precursor** (system output), quantified as the gross calorific value (UHV).

Table 6: Primary energy demand (system boundary level) per 1 kg of product

Primary Energy Demand	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Energy content in polymer precursor [MJ] (energy recovery potential, quantified as gross calorific value of polymer precursor)	41.8	42.4	42.9	42.9	42.9
Process energy [MJ] (quantified as difference between primary energy demand and energy content of polymer precursor)	38.5	23.3	24.7	25.0	14.5
<b>Total primary energy demand (Upper heating value) [MJ]</b>	<b>80.3</b>	<b>65.7</b>	<b>67.6</b>	<b>67.9</b>	<b>57.4</b>
Total primary energy demand (Lower heating value) [MJ]	75.4	61.8	63.6	63.9	53.9

Consequently, the difference ( $\Delta$ ) between primary energy input and energy content in polymer precursor 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 7 to Table 11 show 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 carbon backbone of the polymer precursors – all feedstocks used contain more hydrogen than needed for the polymer precursors considered. Remaining hydrogen is used as process energy. Note that some feedstock input may still be valorised as energy; furthermore, process energy requirements may also be affected by exo-

thermic or endothermic 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).

*Table 7: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg benzene*

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.47	0.024		0.47
Oil	65.23	1.424	45.30	19.93
Natural gas	12.89	0.279	5.55	7.34
Lignite	0.40	0.038		0.40
Nuclear	0.99	0.000		0.99
Other non-renewable fuels	0.00			0.00
Biomass	0.12			0.12
Hydro	0.14			0.14
Solar	0.00			0.00
Geothermics	0.00			0.00
Wind	0.04			0.04
Other renewable fuels	0.00			0.00
<b>Sub-total renewable</b>	<b>0.3</b>	<b>0.0</b>	<b>0.0</b>	<b>0.3</b>
<b>Sub-total Non-renewable</b>	<b>80.0</b>	<b>1.8</b>	<b>50.8</b>	<b>29.1</b>
<b>Total</b>	<b>80.3</b>	<b>1.8</b>	<b>50.8</b>	<b>29.4</b>

*Table 8: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg toluene*

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.29	0.014		0.29
Oil	57.03	1.245	47.08	9.96
Natural gas	7.42	0.161	2.42	5.00
Lignite	0.25	0.024		0.25
Nuclear	0.60	0.000		0.60
Other non-renewable fuels	0.00			0.00
Biomass	0.06			0.06
Hydro	0.08			0.08
Solar	0.00			0.00
Geothermics	0.00			0.00
Wind	0.02			0.02
Other renewable fuels	0.00			0.00
<b>Sub-total renewable</b>	<b>0.2</b>	<b>0.0</b>	<b>0.0</b>	<b>0.2</b>
<b>Sub-total Non-renewable</b>	<b>65.6</b>	<b>1.4</b>	<b>49.5</b>	<b>16.1</b>
<b>Total</b>	<b>65.7</b>	<b>1.4</b>	<b>49.5</b>	<b>16.2</b>

Table 9: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg p-xylene

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.31	0.015		0.31
Oil	60.12	1.313	48.03	12.08
Natural gas	6.11	0.132	1.13	4.98
Lignite	0.28	0.027		0.28
Nuclear	0.65	0.000		0.65
Other non-renewable fuels	0.00			0.00
Biomass	0.06			0.06
Hydro	0.09			0.09
Solar	0.00			0.00
Geothermics	0.00			0.00
Wind	0.02			0.02
Other renewable fuels	0.00			0.00
<b>Sub-total renewable</b>	<b>0.2</b>	<b>0.0</b>	<b>0.0</b>	<b>0.2</b>
<b>Sub-total Non-renewable</b>	<b>67.5</b>	<b>1.5</b>	<b>49.2</b>	<b>18.3</b>
<b>Total</b>	<b>67.6</b>	<b>1.5</b>	<b>49.2</b>	<b>18.5</b>

Table 10: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg o-xylene

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.31	0.015		0.31
Oil	60.39	1.318	48.03	12.35
Natural gas	6.15	0.133	1.13	5.02
Lignite	0.28	0.027		0.28
Nuclear	0.65	0.000		0.65
Other non-renewable fuels	0.00			0.00
Biomass	0.06			0.06
Hydro	0.09			0.09
Solar	0.00			0.00
Geothermics	0.00			0.00
Wind	0.02			0.02
Other renewable fuels	0.00			0.00
<b>Sub-total renewable</b>	<b>0.2</b>	<b>0.0</b>	<b>0.0</b>	<b>0.2</b>
<b>Sub-total Non-renewable</b>	<b>67.8</b>	<b>1.5</b>	<b>49.2</b>	<b>18.6</b>
<b>Total</b>	<b>67.9</b>	<b>1.5</b>	<b>49.2</b>	<b>18.8</b>

Table 11: Analysis by primary energy resources (system boundary level), expressed as energy and/or mass (as applicable) per 1 kg mixed xylenes

Primary energy resource input	Total Energy Input [MJ]	Total Mass Input [kg]	Feedstock Energy Input [MJ]	Fuel Energy Input [MJ]
Coal	0.18	0.009		0.18
Oil	51.55	1.125	48.03	3.51
Natural gas	5.03	0.109	1.13	3.90
Lignite	0.16	0.016		0.16
Nuclear	0.38	0.000		0.38
Other non-renewable fuels	0.00			0.00
Biomass	0.03			0.03
Hydro	0.05			0.05
Solar	0.00			0.00
Geothermics	0.00			0.00
Wind	0.01			0.01
Other renewable fuels	0.00			0.00
<b>Sub-total renewable</b>	<b>0.1</b>	<b>0.0</b>	<b>0.0</b>	<b>0.1</b>
<b>Sub-total Non-renewable</b>	<b>57.3</b>	<b>1.3</b>	<b>49.2</b>	<b>8.1</b>
<b>Total</b>	<b>57.4</b>	<b>1.3</b>	<b>49.2</b>	<b>8.2</b>

Table 12 shows that nearly all of the primary energy demand is from non-renewable resources. Table 13 analyses the types of useful energy inputs in the foreground process: electricity has a minor contribution, whereas the majority is thermal energy (heat). It should be noted, however, that the LCI tables in the electronic datasets account for the entire cradle-to-gate primary energy demand of the considered production system.

Table 12: Primary energy demand by renewability

Fuel/energy input type	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Renewable energy resources	0.4%	0.2%	0.2%	0.2%	0.1%
Non-renewable energy resources	99.6%	99.8%	99.8%	99.8%	99.9%
<b>Total</b>	<b>100.0%</b>	<b>100.0%</b>	<b>100.0%</b>	<b>100.0%</b>	<b>100.0%</b>

Table 13: Analysis by type of useful energy for foreground processes (aromatic complex) per 1 kg of product

Type of useful energy in process input	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Electricity [MJ]	0.14	0.064	0.24	0.24	0.006
Heat, thermal energy [MJ]	4.8	3.4	8.1	8.3	0.47
<b>Total (for selected key processes) [MJ]</b>	<b>5.0</b>	<b>3.5</b>	<b>8.3</b>	<b>8.6</b>	<b>0.48</b>

## Water Consumption

Table 14 shows the gross water resources used in the aromatics production (foreground process).

Table 14: Gross water resources used in foreground processes (aromatic complex) per 1 kg of product

Water use	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Process water [kg]	0.94	0.99	0.75	0.81	0.40
Cooling water [kg]	10.4	15.1	6.6	6.9	0.59
<b>Total [kg]</b>	<b>11.3</b>	<b>16.1</b>	<b>7.4</b>	<b>7.7</b>	<b>0.99</b>

## Air Emission Data

Table 15 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.

Table 15: Selected air emissions from foreground processes (aromatic complex) per 1 kg of product

Air emissions	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Carbon dioxide, fossil [kg]	0.32	0.24	0.52	0.54	0.033
Carbon monoxide (CO) [kg]	$9.3 \times 10^{-5}$	$5.9 \times 10^{-5}$	$1.5 \times 10^{-4}$	$1.5 \times 10^{-4}$	$8.2 \times 10^{-6}$
Sulphur dioxide (SO <sub>2</sub> ) [kg]	$1.6 \times 10^{-3}$	$1.1 \times 10^{-3}$	$1.7 \times 10^{-3}$	$1.7 \times 10^{-3}$	$1.5 \times 10^{-4}$
Nitrogen oxides (NO <sub>x</sub> ) [kg]	$3.6 \times 10^{-4}$	$2.8 \times 10^{-4}$	$5.7 \times 10^{-4}$	$5.9 \times 10^{-4}$	$4.0 \times 10^{-5}$
Particulate matter ≤ 10 µm [kg]	$2.3 \times 10^{-5}$	$4.2 \times 10^{-5}$	$3.0 \times 10^{-5}$	$3.4 \times 10^{-5}$	$6.4 \times 10^{-6}$

## Wastewater Emissions

Table 16 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 16: Selected water emissions from foreground processes (aromatic complex) per 1 kg of product

Water emissions	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
Biological oxygen demand after 5 days (BOD 5) [kg]	$4.2 \times 10^{-6}$	$7.4 \times 10^{-6}$	$5.2 \times 10^{-6}$	$6.0 \times 10^{-6}$	$1.2 \times 10^{-6}$
Chemical oxygen demand (COD) [kg]	$4.8 \times 10^{-5}$	$9.5 \times 10^{-5}$	$1.0 \times 10^{-4}$	$1.1 \times 10^{-4}$	$7.3 \times 10^{-5}$
Total organic carbon (TOC) [kg]	$4.8 \times 10^{-6}$	$8.8 \times 10^{-6}$	$6.1 \times 10^{-6}$	$7.0 \times 10^{-6}$	$1.4 \times 10^{-6}$

## Solid Waste

Table 17 shows the solid waste arising in the aromatics production (foreground process).

Table 17: *Solid waste generation in foreground processes (aromatic complex) per 1 kg of product.*

Product	Unspecified waste for – Incineration kg	Landfill kg	Recovery kg	Unspecified kg	Total kg
Benzene	$3.6 \times 10^{-6}$	0	$2.2 \times 10^{-4}$	0	$2.2 \times 10^{-4}$
Toluene	$6.6 \times 10^{-6}$	0	$3.7 \times 10^{-4}$	0	$3.8 \times 10^{-4}$
p-Xylene	$4.6 \times 10^{-6}$	0	$2.8 \times 10^{-4}$	0	$2.8 \times 10^{-4}$
o-Xylene	$5.3 \times 10^{-6}$	0	$3.1 \times 10^{-4}$	0	$3.2 \times 10^{-4}$
Mixed Xylenes	$9.9 \times 10^{-7}$	0	$9.2 \times 10^{-5}$	0	$9.3 \times 10^{-5}$

# 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 2010].

Table 18: Abiotic Depletion Potential (ADP) per 1 kg of product

Natural resources	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
ADP, elements [kg Sb eq]	$4.6 \times 10^{-8}$	$3.8 \times 10^{-8}$	$3.5 \times 10^{-8}$	$3.6 \times 10^{-8}$	$2.7 \times 10^{-8}$
ADP, fossil fuels (LHV) [MJ]	74.1	61.0	62.8	63.1	53.5

## 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 basing on the last report of the Intergovernmental Panel on Climate Change [IPCC 2007].

Table 19: Global Warming Potential (GWP, 100 years) per 1 kg of product

Climate change	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
GWP [kg CO <sub>2</sub> eq.]	1.86	1.22	1.43	1.45	0.79

### Acidification

The Acidification Potential (AP) is quantified according to HAUSCHILD 1998 with updated characterisation factors of CML [CML 2010].

Table 20: Acidification Potential per 1 kg of product

Acidification of soils and water bodies	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
AP [g SO <sub>2</sub> eq.]	6.12	4.75	5.70	5.80	3.23

## Eutrophication

The Eutrophication Potential (EP) is calculated according to HEIJUNGS 1992 with updated characterisation factors of CML [CML 2010].

Table 21: Eutrophication Potential per 1 kg of product

Eutrophication of soils and water bodies	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
EP, terrestrial [g PO <sub>4</sub> <sup>3-</sup> eq.]	0.42	0.33	0.37	0.38	0.25
EP, aquatic [g PO <sub>4</sub> <sup>3-</sup> eq.]	0.84	0.73	0.77	0.77	0.66
EP, total [g PO <sub>4</sub> <sup>3-</sup> eq.]	1.26	1.06	1.14	1.15	0.91

## 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 dinitrogen monoxide (N<sub>2</sub>O) as ozone depleting substance with an ODP of 0.017 kg CFC-11 eq. per kg of N<sub>2</sub>O. This emission plays a relevant role for the overall ODP result of the considered products in this study with 23 % to 37 %.

Table 22: Ozone Depletion Potential per 1 kg of product

Ozone Depletion Potential	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
ODP [g CFC-11 eq.]	5.2 x 10 <sup>-4</sup>	4.1 x 10 <sup>-4</sup>	5.6 x 10 <sup>-4</sup>	5.7 x 10 <sup>-4</sup>	2.7 x 10 <sup>-4</sup>

## Summer Smog

The Photochemical Ozone Creation Potential (POCP) is quantified according to JENKIN 1999 and DERWENT 1998 with updated characterisation factors of CML [CML 2010].

Table 23: Photochemical Ozone Creation Potential per 1 kg of product

Photochemical Ozone Creation Potential	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
POCP [g Ethene eq.]	0.40	0.28	0.29	0.29	0.18

## Dust & Particulate Matter

Particulate matter with an aerodynamic diameter of less than 10 µm (PM<sub>10</sub>) is suspected to cause heart and circulatory diseases. New studies from internationally recognised organisations (e.g. WHO 2006) confirm a high mortality risk from fine dust.

Large scale air pollution of PM<sub>10</sub> is caused by direct emissions of particulate matter and secondary particles that are formed by precursors such as nitrogen dioxide (NO<sub>2</sub>), sulphur dioxide (SO<sub>2</sub>), ammonia (NH<sub>3</sub>) and Non-Methane Volatile Organic Compounds (NMVOC). The characterisation factors shown in Table 24 are based on works of DE LEEUW 2002 and HELDSTAB 2003 for NMVOC.

Table 24: *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
Secondary aerosol formers (precursors)	
NO <sub>x</sub> (as NO <sub>2</sub> )	0.88
SO <sub>2</sub>	0.54
NH <sub>3</sub>	0.64
NMVOC	0.012

Table 25: *PM10 emissions per 1 kg polymer precursor*

Particulate matter ≤ 10 µm	Benzene	Toluene	p-Xylene	o-Xylene	Mixed Xylenes
PM10, direct emissions [PM10 eq.]	0.27	0.24	0.24	0.25	0.18
PM10, secondary [PM10 eq.]	4.85	3.77	4.45	4.52	2.68
PM10, total [PM10 eq.]	5.12	4.01	4.69	4.77	2.87

## Dominance Analysis

Table 26 to 30 show the main contributions to the results presented above.

Table 26: *Dominance analysis of impacts per 1 kg benzene*

	Total Primary Energy <sup>a)</sup>	ADP Elements	ADP Fossil <sup>a)</sup>	GWP	AP	EP	POCP	PM10
	[MJ]	[kg Sb eq.]	[MJ]	[kg CO <sub>2</sub> eq.]	[g SO <sub>2</sub> eq.]	[g PO <sub>4</sub> <sup>3-</sup> eq.]	[g Ethene eq.]	[g PM10 eq.]
<b>Foreground processes</b> (aromatics complex) incl. thermal energy	0.0%	26.7%	0.0%	17.6%	30.1%	4.3%	22.6%	23.4%
<b>Electricity</b> for foreground processes	0.5%	0.5%	0.3%	1.0%	1.1%	0.4%	0.6%	1.0%
<b>Steam Cracking</b> (pyrolysis gasoline)	1.8%	13.7%	0.9%	35.6%	7.2%	5.2%	34.4%	9.3%
<b>Refinery</b>	0.0%	55.3%	0.0%	22.7%	18.1%	4.6%	14.0%	16.1%
<b>Crude oil &amp; Natural gas</b> extraction and transport	97.7%	3.7%	98.8%	23.2%	43.4%	85.6%	28.4%	50.2%
<b>Process waste treatment</b>	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
<b>Total</b>	100%	100%	100%	100%	100%	100%	100%	100%

<sup>a)</sup> Due to the supply chain of feedstock, the resource depletion is ultimately assigned to crude oil and natural gas activities. The distribution would be different if useful energy was considered.

Table 27: Dominance analysis of impacts per 1 kg toluene

	Total Primary Energy <sup>a)</sup>	ADP Elements	ADP Fossil <sup>a)</sup>	GWP	AP	EP	POCP	PM10
	[MJ]	[kg Sb eq.]	[MJ]	[kg CO <sub>2</sub> eq.]	[g SO <sub>2</sub> eq.]	[g PO <sub>4</sub> <sup>3-</sup> eq.]	[g Ethene eq.]	[g PM10 eq.]
<b>Foreground processes</b> (aromatics complex) incl. thermal energy	0.0%	37.1%	0.0%	19.8%	27.8%	4.3%	26.4%	22.3%
<b>Electricity</b> for foreground processes	0.3%	0.3%	0.2%	0.7%	0.7%	0.2%	0.4%	0.6%
<b>Steam Cracking</b> (pyrolysis gasoline)	1.0%	7.5%	0.5%	24.3%	4.2%	2.8%	22.2%	5.3%
<b>Refinery</b>	0.0%	51.2%	0.0%	25.4%	19.6%	4.3%	16.9%	17.0%
<b>Crude oil &amp; Natural gas</b> extraction and transport	98.7%	3.9%	99.3%	29.8%	47.7%	88.4%	34.1%	54.7%
<b>Process waste treatment</b>	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
<b>Total</b>	100%	100%	100%	100%	100%	100%	100%	100%

<sup>a)</sup> Due to the supply chain of feedstock, the resource depletion is ultimately assigned to crude oil and natural gas activities. The distribution would be different if useful energy was considered.

Table 28: Dominance analysis of impacts per 1 kg p-xylene

	Total Primary Energy <sup>a)</sup>	ADP Elements	ADP Fossil <sup>a)</sup>	GWP	AP	EP	POCP	PM10
	[MJ]	[kg Sb eq.]	[MJ]	[kg CO <sub>2</sub> eq.]	[g SO <sub>2</sub> eq.]	[g PO <sub>4</sub> <sup>3-</sup> eq.]	[g Ethene eq.]	[g PM10 eq.]
<b>Foreground processes</b> (aromatics complex) incl. thermal energy	0.0%	31.1%	0.0%	37.0%	36.1%	7.3%	36.8%	30.4%
<b>Electricity</b> for foreground processes	1.0%	1.1%	0.5%	2.1%	2.0%	0.7%	1.3%	1.9%
<b>Steam Cracking</b> (pyrolysis gasoline)	0.5%	3.8%	0.2%	9.8%	1.6%	1.2%	10.1%	2.2%
<b>Refinery</b>	0.0%	59.6%	0.0%	24.6%	18.8%	4.5%	18.1%	16.8%
<b>Crude oil &amp; Natural gas</b> extraction and transport	98.5%	4.3%	99.2%	26.4%	41.4%	86.2%	33.7%	48.8%
<b>Process waste treatment</b>	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
<b>Total</b>	100%	100%	100%	100%	100%	100%	100%	100%

<sup>a)</sup> Due to the supply chain of feedstock, the resource depletion is ultimately assigned to crude oil and natural gas activities. The distribution would be different if useful energy was considered.

Table 29: Dominance analysis of impacts per 1 kg o-xylene

	<b>Total Primary Energy<sup>a)</sup></b>	<b>ADP Elements</b>	<b>ADP Fossil<sup>a)</sup></b>	<b>GWP</b>	<b>AP</b>	<b>EP</b>	<b>POCP</b>	<b>PM10</b>
	[MJ]	[kg Sb eq.]	[MJ]	[kg CO <sub>2</sub> eq.]	[g SO <sub>2</sub> eq.]	[g PO <sub>4</sub> <sup>3-</sup> eq.]	[g Ethene eq.]	[g PM10 eq.]
<b>Foreground processes</b> (aromatics complex) incl. thermal energy	0.0%	32.8%	0.0%	37.8%	37.0%	7.6%	37.6%	31.2%
<b>Electricity</b> for foreground processes	1.0%	1.1%	0.5%	2.1%	2.0%	0.7%	1.3%	1.9%
<b>Steam Cracking</b> (pyrolysis gasoline)	0.5%	3.7%	0.2%	9.7%	1.6%	1.2%	10.0%	2.1%
<b>Refinery</b>	0.0%	58.2%	0.0%	24.3%	18.5%	4.5%	17.8%	16.5%
<b>Crude oil &amp; Natural gas</b> extraction and transport	98.5%	4.2%	99.2%	26.1%	40.9%	86.0%	33.3%	48.2%
<b>Process waste treatment</b>	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
<b>Total</b>	100%	100%	100%	100%	100%	100%	100%	100%

<sup>a)</sup> Due to the supply chain of feedstock, the resource depletion is ultimately assigned to crude oil and natural gas activities. The distribution would be different if useful energy was considered.

Table 30: Dominance analysis of impacts per 1 kg mixed xylenes

	<b>Total Primary Energy<sup>a)</sup></b>	<b>ADP Elements</b>	<b>ADP Fossil<sup>a)</sup></b>	<b>GWP</b>	<b>AP</b>	<b>EP</b>	<b>POCP</b>	<b>PM10</b>
	[MJ]	[kg Sb eq.]	[MJ]	[kg CO <sub>2</sub> eq.]	[g SO <sub>2</sub> eq.]	[g PO <sub>4</sub> <sup>3-</sup> eq.]	[g Ethene eq.]	[g PM10 eq.]
<b>Foreground processes</b> (aromatics complex) incl. thermal energy	0.0%	22.0%	0.0%	4.5%	5.6%	0.9%	14.7%	4.3%
<b>Electricity</b> for foreground processes	0.0%	0.0%	0.0%	0.1%	0.1%	0.0%	0.0%	0.1%
<b>Steam Cracking</b> (pyrolysis gasoline)	0.5%	4.4%	0.2%	15.6%	2.5%	1.3%	14.1%	3.1%
<b>Refinery</b>	0.0%	68.6%	0.0%	39.1%	29.1%	5.0%	25.3%	24.1%
<b>Crude oil &amp; Natural gas</b> extraction and transport	99.5%	4.9%	99.7%	40.8%	62.7%	92.7%	45.9%	68.5%
<b>Process waste treatment</b>	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
<b>Total</b>	100%	100%	100%	100%	100%	100%	100%	100%

<sup>a)</sup> Due to the supply chain of feedstock, the resource depletion is ultimately assigned to crude oil and natural gas activities. The distribution would be different if useful energy was considered.

## Comparison of the Present Eco-profile with its Previous Version

The primary energy demand (PED) for benzene production is significantly higher than for toluene or xylenes production (see Table 6). For mixed xylenes the PED is even lower. This is a result of the following:

- The two feedstocks for aromatics production have different 'burdens': pyrolysis gasoline which is a product of steam cracking of naphtha (predominantly) has a higher primary energy demand than reformat (72.6 MJ/kg and 51.9 MJ/kg, respectively). There is a similar difference for GWP: pyrolysis gasoline 1.44 kg CO<sub>2</sub>e/kg compared with reformat 0.57 kg CO<sub>2</sub>e/kg.
- As shown in Table 2, benzene is mostly produced from pyrolysis gasoline (61 %), whereas toluene and xylenes are produced mostly from reformat (70 and 86 %, respectively).
- Benzene is also produced by hydrodealkylation of toluene and xylenes, which is a highly energy-intensive process.
- 'Mixed xylenes' is a mixture of different xylenes, only separated from lower and higher aromatics, and from alkanes. Thus, no energy-intensive separation steps are included.

The differences between the products under investigation are less pronounced regarding the emissions, except for CO<sub>2</sub>/GWP. This is a result of the complex mixture of a) two different feedstocks and b) different fuels burned in the different productions phases: in the refinery, more heavy fuel-oil based fuels are used with higher specific emissions of CO<sub>2</sub>, NO<sub>x</sub> and SO<sub>2</sub>; whereas in the aromatics complex, light ends from internal processes (i.e. methane, ethane, and hydrogen) are burned with comparably lower specific emissions.

Table 31 to 35 compare the present results with the previous version of the Eco-profile of 2005. Care has to be taken when deriving an interpretation, because some methodological aspects of the previous study were not transparently reported, and detailed information regarding the inclusion of pyrolysis gasoline (with significantly higher primary energy demand) as feedstock to the aromatics complex was not provided: "The principal route for the commercial production of benzene is catalytic reforming. (...) In some plants the naphtha feed may be replaced by the pyrolysis gasoline fraction from naphtha cracking"[BOUSTEAD 2005]. Therefore, the possibility of meaningful comparison of the current and previous results is very limited. Energy demand and GWP for benzene production was calculated to be significantly higher than previously reported. This is most likely due to the fact that pyrolysis gasoline was now considered to be the main feedstock for benzene production. Differences are smaller for toluene and xylenes, most likely due to their reformat-based feedstock.

Table 31: Comparison of the present Eco-profile of benzene with its previous version (2002/2005)

Environmental Impact Categories	Benzene Eco-profile Process data 2002 Calculated 2005	Benzene Eco-profile 2013	Difference
Gross primary energy from resources [MJ]	64.7	80.3	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] <sup>(a)</sup>	$3.6 \times 10^{-8}$	$4.6 \times 10^{-8}$	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	63.3	74.1	Direct comparison is not possible: the energy intensive production route via steam cracker was most likely not considered in previous Eco-profile
Global Warming Potential (GWP) [kg CO <sub>2</sub> eq.]	1.76	1.86	
Acidification Potential (AP) [g SO <sub>2</sub> eq.] <sup>(a)</sup>	6.3	6.1	
Eutrophication Potential (EP) [g PO <sub>4</sub> <sup>3-</sup> eq.] <sup>(a)</sup>	0.43	1.3	
Ozone Depletion Potential (ODP) [g CFC-11 eq.] <sup>(a)</sup>	$2.8 \times 10^{-6}$	$5.2 \times 10^{-4}$	
Photochemical Ozone Creation Potential [g Ethene eq.] <sup>(a)</sup>	0.36	0.40	

<sup>a)</sup> Results are not included in previous Eco-profile; values have been extracted from implemented dataset in ecoinvent v2.2

Table 32: Comparison of the present Eco-profile of toluene with its previous version (2002/2005)

Environmental Impact Categories	Toluene Eco-profile Process data 2002 Calculated 2005	Toluene Eco-profile 2012	Difference
Gross primary energy from resources [MJ]	61.5	65.7	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] <sup>(a)</sup>	$2.8 \times 10^{-8}$	$3.8 \times 10^{-8}$	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	60.5	61.0	Direct comparison is not possible: the energy intensive production route via steam cracker was most likely not considered in previous Eco-profile
Global Warming Potential (GWP) [kg CO <sub>2</sub> eq.]	1.48	1.22	
Acidification Potential (AP) [g SO <sub>2</sub> eq.] <sup>(a)</sup>	3.8	4.7	
Eutrophication Potential (EP) [g PO <sub>4</sub> <sup>3-</sup> eq.] <sup>(a)</sup>	0.32	1.1	
Ozone Depletion Potential (ODP) [g CFC-11 eq.] <sup>(a)</sup>	$1.8 \times 10^{-6}$	$4.1 \times 10^{-4}$	
Photochemical Ozone Creation Potential [g Ethene eq.] <sup>(a)</sup>	0.24	0.28	

<sup>a)</sup> Results are not included in previous Eco-profile; values have been extracted from implemented dataset in ecoinvent v2.2

Table 33: Comparison of the present Eco-profile of p-xylene with its previous version (2002/2005)

Environmental Impact Categories	Xylene Eco-profile Process data 2002 Calculated 2005	p-Xylene Eco-profile 2012	Difference
Gross primary energy from resources [MJ]	64.0	67.6	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] <sup>(a)</sup>	$2.9 \times 10^{-8}$	$3.5 \times 10^{-8}$	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	62.7	62.8	Direct comparison is not possible: the energy intensive production route via steam cracker was most likely not considered in previous Eco-profile
Global Warming Potential (GWP) [kg CO <sub>2</sub> eq.]	1.61	1.43	
Acidification Potential (AP) [g SO <sub>2</sub> eq.] <sup>(a)</sup>	4.5	5.7	
Eutrophication Potential (EP) [g PO <sub>4</sub> <sup>3-</sup> eq.] <sup>(a)</sup>	0.37	1.1	
Ozone Depletion Potential (ODP) [g CFC-11 eq.] <sup>(a)</sup>	$2.0 \times 10^{-6}$	$5.6 \times 10^{-4}$	
Photochemical Ozone Creation Potential [g Ethene eq.] <sup>(a)</sup>	0.28	0.29	

<sup>a)</sup> Results are not included in previous Eco-profile; values have been extracted from implemented dataset in ecoinvent v2.2

Table 34: Comparison of the present Eco-profile of o-xylene with its previous version (2002/2005)

Environmental Impact Categories	Xylene Eco-profile Process data 2002 Calculated 2005	o-Xylene Eco-profile 2012	Difference
Gross primary energy from resources [MJ]	64.0	67.9	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] <sup>(a)</sup>	$2.9 \times 10^{-8}$	$3.6 \times 10^{-8}$	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	62.7	63.1	Direct comparison is not possible: the energy intensive production route via steam cracker was most likely not considered in previous Eco-profile
Global Warming Potential (GWP) [kg CO <sub>2</sub> eq.]	1.61	1.45	
Acidification Potential (AP) [g SO <sub>2</sub> eq.] <sup>(a)</sup>	4.5	5.8	
Eutrophication Potential (EP) [g PO <sub>4</sub> <sup>3-</sup> eq.] <sup>(a)</sup>	0.37	1.2	
Ozone Depletion Potential (ODP) [g CFC-11 eq.] <sup>(a)</sup>	$2.0 \times 10^{-6}$	$5.7 \times 10^{-4}$	
Photochemical Ozone Creation Potential [g Ethene eq.] <sup>(a)</sup>	0.28	0.29	

<sup>a)</sup> Results are not included in previous Eco-profile; values have been extracted from implemented dataset in ecoinvent v2.2

Table 35: Comparison of the present Eco-profile of mixed xylenes with its previous version (2002/2005)

Environmental Impact Categories	Xylene Eco-profile Process data 2002 Calculated 2005	Mixed Xylenes Eco-profile 2012	Difference
Gross primary energy from resources [MJ]	64.0	57.4	
Abiotic Depletion Potential (ADP), elements [kg Sb eq.] <sup>(a)</sup>	$2.9 \times 10^{-8}$	$2.7 \times 10^{-8}$	
Abiotic Depletion Potential (ADP), fossil fuels [MJ]	62.7	53.5	Direct comparison is not possible: the energy intensive production route via steam cracker was most likely not considered in previous Eco-profile
Global Warming Potential (GWP) [kg CO <sub>2</sub> eq.]	1.61	0.79	
Acidification Potential (AP) [g SO <sub>2</sub> eq.] <sup>(a)</sup>	4.5	3.2	
Eutrophication Potential (EP) [g PO <sub>4</sub> <sup>3-</sup> eq.] <sup>(a)</sup>	0.37	0.9	
Ozone Depletion Potential (ODP) [g CFC-11 eq.] <sup>(a)</sup>	$2.0 \times 10^{-6}$	$2.7 \times 10^{-4}$	
Photochemical Ozone Creation Potential [g Ethene eq.] <sup>(a)</sup>	0.28	0.18	

<sup>a)</sup> Results are not included in previous Eco-profile; values have been extracted from implemented dataset in ecoinvent v2.2

# Review

## Review Details

The goal and scope of this Eco-profile study was confirmed to be a European production average of the following polymer precursors: benzene, toluene, and ortho-, para-, and mixed xylenes (BTX). The geographical scope includes the EU 27 member states and Norway. Benchmarking data for 50 European steam cracker units were complemented by a desktop study of upstream operations (extraction, refinery), aromatics separation unit, and alternative routes (catalytic reformer, hydrodealkylation). The technological scope probably differs somewhat from the previous versions of the BTX Eco-profiles published by PlasticsEurope which had presumably been limited to catalytic reforming, but were insufficiently transparent on this issue.

The main data source used for this study was a validated confidential report by the petrochemical industry (APPE) under the European Emission Trading Scheme (ETS) on energy use and CO<sub>2</sub> emissions of European steamcracking operations. Other processes, including refinery, catalytic reformer, and hydrodealkylation, were derived from proprietary models (developed by the practitioner IFEU through various petrochemical industry projects). Further, publicly available literature data were used. The review confirmed that, despite no primary data was collected, the data used are applicable, up-to-date, and modelled with a view to internal consistency. The temporal scope was confirmed to be 2010 as reference year and valid at least until 2014 in view of the slow technological changes.

The following aspects were subject to particular scrutiny by the review panel:

- The shares of the alternative routes: extraction from pyrolysis gasoline, catalytic reforming of naphtha, HDA of toluene, coking and HDA of other aromatics;
- the modelling of raffinate (saturated hydrocarbons) as by-product;
- the differences in specific resource use and emissions assigned to the various BTX;
- the consistent and justifiable use of allocation methods;
- plausibility checks of calculations along the productions chains.

A review meeting between the LCA practitioner and the reviewers was held, including a model and database review, and spot checks of data and calculations. The results are thus held to be representative and reliable for the specified production routes. It is noteworthy that, compared with previous studies under the PlasticsEurope Eco-profiles programme, the results for benzene and mixed xylenes have changed notably:

- The previous edition of the Eco-profiles for cracker products apparently used a mass allocation of energy demand and emissions of the steam cracking process to all cracker output streams (thus lowering specific burdens), not only to the HVC as in the present version; from today's perspective, also to ensure consistency with current industry practice (APPE), the allocation used here is deemed more appropriate.
- According to recent industry data (APPE), benzene is predominantly (approx. 60%) produced from pygas, whereas other aromatics are predominantly (>70%) produced from reformate. Since the pygas route has higher burdens than the reformer route, indicators for benzene have increased.
- Conversely, mixed xylenes were shown to require less steam for separation than o- and p-xylene. As a result, the indicators for mixed xylenes have decreased.

- It is noteworthy that fuel-grade by-products, specifically raffinate (saturated hydrocarbons), were calculated with their calorific value and with their upstream burdens (oil extraction, transport and refining), but no process-related environmental impacts were assigned to them. Process-related burdens (steamcracking, aromatics separation) were only allocated to the high-value BTX compounds.
- The overall levels of greenhouse gas emissions of the steam cracker and aromatics units were confirmed to be in line with APPE's ETS reporting and internal reports. For greenhouse gas emissions, the results of this new version of the Eco-profile are quite in line with the previous versions of 2005 (with the noteworthy exception of benzene and mixed xylenes discussed above).
- Other impact categories changed somewhat in proportion with the process energy requirements. It should be noted, however, that some indicators apparently changed substantially due to life cycle inventory items in the previous version not being specific enough to allow an accurate *a posteriori* calculation (average characterisation factors applied to unspecified substance flows). In these cases, a comparison with the previous version is strictly speaking not valid.

Further, the review verified that the model and calculations comply with the rules of the PlasticsEurope Eco-profiles methodology and with ISO 14040–14044: the resulting life cycle inventory datasets for benzene, toluene, and o-, p-, and mixed xylenes (BTX) are thus compatible building blocks for use in other Eco-profile calculations.

## Review Summary

The Eco-profile of benzene, toluene, and ortho-, para-, and mixed xylenes (BTX) has been validated to appropriately represent current European production of these polymer precursors. The underlying emission data for the steam cracking process are consistent with reports of the petrochemical industry under the European Emission Trading Scheme (ETS). Other processes, including refinery, catalytic reformer, and hydrodealkylation were derived from project and literature data and modelled with a view to internal consistency. The results are thus held to be representative and reliable for the specified production routes.

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