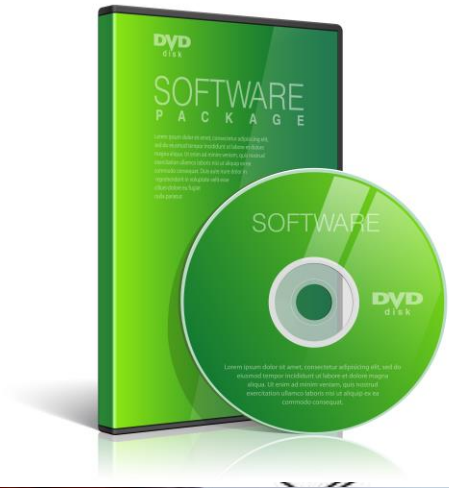

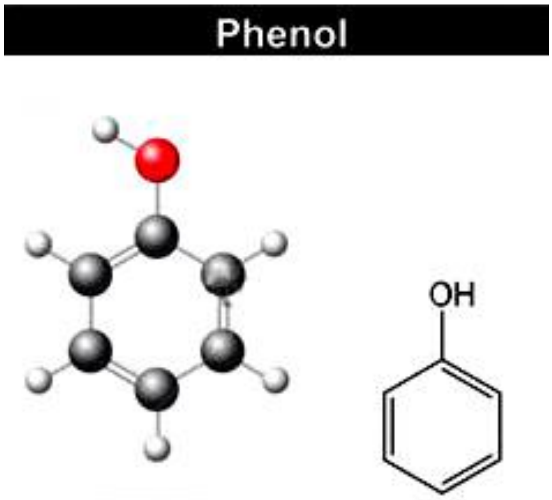

Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers

Phenol and Acetone
CEFIC Petrochemicals Europe – Phenol and Acetone Sector Group
September 2016

PASG - Phenol and Acetone Sector Group

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Environmental Product Declaration

Introduction

This Environmental Product Declaration (EPD) is based upon life cycle inventory (LCI) data from the GaBi database 2015 [GaBi 6]. It has been prepared based on **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) [PlasticsEurope 2011], however, main differences to the requirements set out in this methodology are the following:

- The LCIs for phenol and acetone are not based on primary industry data but solely on literature data complemented with expert knowledge from industry experts (PASG members) and the LCA practitioner;
- Instead of country-specific production conditions based on actual phenol/acetone manufacturing sites, EU-specific datasets for the background system have been used;
- Due to the above, no representativeness statement in the sense of a real European production average can be made.

For the phenol and acetone datasets, no detailed Eco-profile report but only this EPD has been prepared.

EPDs provide environmental performance data, but no information on the economic and social aspects which would be necessary for a complete sustainability assessment. EPDs do not imply a value judgement between environmental criteria.

This EPD describes the production of Phenol and Acetone from cradle to gate (from crude oil extraction to an average plant gate) based on literature information. **Please keep in mind that comparisons cannot be made on the level of the material alone**: it is necessary to consider the full life cycle of an application in order to compare the performance of different materials and the effects of relevant life cycle parameters. This EPD is intended to be used by member companies, to support product-orientated environmental management; by users of such materials, 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	thinkstep AG
LCA Practitioner	thinkstep AG
Programme Owner	PlasticsEurope aisbl
Programme Manager, Reviewer	Schulz Sustainability Consulting on behalf of DEKRA Assurance Services GmbH
Number of plants included in data collection	Secondary data
Representativeness	n.a.
Reference year	2015 (refers to background system)
Year of data collection and calculation	n.a.
Expected temporal validity	2025
Cut-offs	No significant cut-offs
Data Quality	Good
Allocation method	Net calorific value allocation

Description of the Product and the Production Process

The Phenol/Acetone process belongs to NACE code 2414 (Manufacture of other organic basic chemicals, with a production capacity of more than 100 tons per day).

Phenol is mainly used as an intermediate in organic synthesis. In this, phenol essentially serves as a raw material for the production of bisphenol A, phenolic resins, alkylphenols and caprolactam. It is also used for salicylic acid, nitrophenols, diphenyl ethers, halogenated phenols and other chemicals.

Acetone is mainly used as solvent and in the production of methyl methacrylate and bisphenol A. It is a common building block in organic chemistry.

Production Process

Phenol and co-product Acetone are produced via a two-step process starting from cumene (Hock process). In the first step, cumene is oxidized with ambient or enriched air to form cumene hydroperoxide. This step is an autocatalytic oxidation. The hydroperoxide is then concentrated and subsequently decomposed (cleaved) by acid-catalyzed rearrangement into acetone and phenol. The catalyst is subsequently removed and the reactor effluent neutralized before being sent to a fractionation unit.

High-purity phenol and acetone is obtained in a series of purification steps, which may include hydro-extractive distillation, catalytic treatment, and extraction with caustics. The side-products alpha-methyl styrene (AMS) and acetophenone are recovered as useful products in some cases. AMS is usually hydrogenated and recycled back to the hydroperoxidation unit. Other by-products like tars are used as fuel.

The reference flow for Phenol and Acetone, to which all data given in this Eco-profile refer, is 1 kg of the respective product.

Data Sources and Allocation

The main data source is a secondary data research undertaken by thinkstep. Important data sources are:

- Karl Heinz Buchel, Hans-Heinrich Moretto, Dietmar Werner: Industrial Inorganic Chemistry, Wiley-VCH, 2000
- Prof. Dr. Klaus Weissermel, Prof. Dr. Hans-Jürgen Arpe: Industrial Organic Chemistry, Wiley-VCH, 2008
- Manfred Weber, Markus Weber, Michael Kleine-Boymann: Phenol; Ullmann's Encyclopedia of Industrial Chemistry; 2004
- Phenol; Römpp Online, Georg Thieme Verlag, 2013
- PDC B.V., Rule Book for the Phenol/Acetone Sector -v3-, Netherlands, May 19, 2010

The Hock process is well described in these literature sources. The phenol and acetone datasets were developed based on information from these sources coupled with thinkstep‘s chemical engineering know-how.

The background data system is taken from the database of the software system GaBi 6 [GaBi 6] and represents European production conditions.

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

The Hock process forms the products Phenol (57,5% in mass), Acetone (36% in mass), alpha-Methylstyrene (4,1% in mass) and Acetophenone (4,1% in mass). The desired products of the Hock process, described in this environmental product declaration are Phenol and Acetone as marketable products. Most companies use acetophenone for energy generation or sell it as stand-alone product. Alpha-Methylstyrene is often fed back into the cumene input (hydro-peroxidation step), but not necessarily sold as product.

As Phenol and Acetone are valuable products of the Hock Process and the use of Acetophenone and alpha-Methylstyrene do not follow the same paths entirely, an allocation to net calorific value (corresponding to the C-content of the molecules) is applied, although Phenol would generate higher income than Acetone. Applying an allocation by economic value would result in a higher allocation factor for Phenol and higher environmental burden, respectively.

The energy content allocation results in the allocation of environmental burdens as follows:

- 33,8% Acetone
- 59,1% Phenol
- 4,05% Acetophenone
- 3% alpha-Methylstyrene

The previous Eco-Profile on Acetone and Phenol used mass as physical relationship. Following the argumentation above an allocation by energy content is justified as valid.

The full documentation of the LCI data can be found on the GaBi homepage (http://www.gabi-software.com/deutsch/support/gabi/gabi-database-2016-lci-documentation/professional-database-2016/)

Use Phase and End-of-Life Management

Around 37% of global Phenol output is used for the production of bisphenol A. Bisphenol A is especially used for the production of high-grade polycarbonates for compact discs, for glazing, and for the automotive industry. Bisphenol A is also used for the production of epoxy resins.
The second largest consumption of phenol is for the production of phenolic resins with formaldehyde. They are mainly used for underseal applications in the automotive industry. Phenol is also used for the production of caprolactam via cyclohexanol.

The main use of acetone is as a chemical intermediate in the manufacture of acetone cyanohydrin for methyl methacrylate (MMA), bisphenol A, and aldol chemicals like di-acetone alcohol (DAA), mesityl oxide (MOX), and methyl isobutyl ketone (MIBK). Acetone is also used as solvent for a multitude of applications.

Environmental Performance

The tables 1 and 2 below show the environmental performance indicators associated with the production of 1 kg Phenol and 1 kg Acetone.

Input Parameters

Table 1: Input Parameter per 1 kg Acetone and 1 kg Phenol

Indicator	Unit	Acetone	Phenol
Non-renewable energy resources[1)]	MJ	61,08	66,86
• Fuel energy	MJ	29,79	31,22
• Feedstock energy[2)]	MJ	31,28	35,64
Renewable energy resources (biomass)[1)]	MJ	0,79	0,87
• Fuel energy	MJ	0,79	0,87
• Feedstock energy	MJ	0	0
Abiotic Depletion Potential			
• Elements	kg Sb eq	5,35E-07	5,86E-07
• Fossil fuels	MJ	5,54E+01	6,06E+01
Renewable materials (biomass)	kg	0	0
Water use (key foreground process level)	kg	2,05	2,23
• for process	kg	0,31	0,33
• for cooling	kg	1,74	1,90

1) Calculated as upper heating value (UHV)

2) Calculated based on heating value of the product with a surcharge of 10%

Output Parameters

Table 2: Output Parameter per 1 kg Acetone and 1 kg Phenol

Indicator	Unit	Acetone	Phenol
GWP	kg CO_2 eq	1,64	1,79
ODP	g CFC-11 eq	1,06E-07	1,16E-07
AP	g SO_2 eq	3,41	3,73
POCP	g Ethene eq	0,84	0,92
EP	g PO_4 eq	0,32	0,36
Dust/particulate matter (2.5pm - 10 pm)	g PM10	1,05E-01	1,15E-01
Total particulate matter	g	1,39E-01	1,52E-01
Waste			
• Radioactive waste	kg	4,06E-04	4,44E-04
• Non-radioactive waste [3)]	kg	7,63E-03	8,35E-03

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

Additional Environmental and Health Information

ETS Rule Book

The existing LCA model for the Hock Process resulting in the marketable products Acetone and Phenol was checked against data retrieved from the ETS rule book for phenol and acetone production. The comparison revealed that the assumed system boundaries and the product mix of phenol, acetone, alphamethyl styrene and acetophenone are comparable. Especially, the stated CO_2 emissions caused by electricity and thermal energy by the ETS rule book were synchronized with the LCA model and only minor differences were found. Most likely these differences result from multiple reference years of used emission profiles for energy supply such as electricity and thermal energy.
As the ETS rule book does not cover any upstream emissions of cumene, auxiliary products and fuel exploration (used for steam and electricity generation), these emission profiles could not be compared with the LCA model used for this analysis.

REACH regulation

A “Phenol & Acetone” REACH Consortium was formed through which manufacturers have joined efforts to prepare by 30 November 2010 consistent registration dossiers covering phenol and its derivative substances including phenol, acetone, cumene, alphamethyl styrene, acetophenone, di-isopropyl benzene, and "high boiler".

Dominance Analysis

Table 3 shows the main contributions to the results presented above. Although the absolute results are different for 1 kg Phenol or 1 kg Acetone, the relative contribution is the same due to the used allocation approach (allocation by energy content). For both products, the precursor cumene dominates with 59% to 86% of the overall impact in all analysed environmental impact categories, except ODP.

The group “Process chemicals and auxiliaries” covers nitrogen, soda, sodium hydroxide and sulphuric acid supply, which show significant influence to the category ADP elements. Direct process emissions from the Hock Process are covered in the group process emissions which contributes for 8% to the total POCP – smog formation.

Moreover, the contribution to total energy supply, electrical and thermal energy of the considered foreground production process contributes to a significant share in all impact categories, especially for steam supply with 22% contribution in GWP and electricity supply with 48% in ODP.

Table 3: Dominance analysis of impacts per 1 kg Phenol or 1 kg Acetone

	Total Primary Energy [MJ]	ADP Elements [kg Sb eq.]	ADP Fossil [MJ]	GWP [kg CO_2 eq.]	AP [g SO_2 eq.]	EP [g PO_4^{3-} eq]	ODP [g CFC-11 eq]	POCP [g Ethene eq.]
Cumene	86%	59%	87%	72%	85%	80%	42%	82%
Process water supply	0%	16%	0%	1%	1%	1%	2%	0%
Process chemicals and auxiliaries	0%	18%	0%	1%	2%	1%	4%	2%
Process emissions	0%	0%	0%	0%	0%	1%	0%	8%
Steam supply	10%	2%	11%	22%	7%	11%	5%	6%
Electricity supply	3%	4%	1%	4%	6%	6%	48%	2%
Waste incineration and waste water treatment	0%	0%	0%	0%	0%	0%	0%	0%
Total	100%	100%	100%	100%	100%	100%	100%	100%

Comparison of the Present Eco-profile with its Previous Version (2005)

In 2005, an Eco-profile of acetone and phenol was carried out by I. Boustead based on primary production data from 1994 [BOUSTEAD 2005].

Unfortunately, no detailed information on foreground data and applied background LCIs is available to enable precise comparison with the current Eco-profile. Finally, in that past Eco-profile, the results consisted mostly of partial life cycle inventory (LCI) results that are too sparse to be reused to calculate a comparative LCIA.

However, even considering the above restrictions, two final life cycle impact assessment (LCIA) results reported in 2005 are still partly methodologically consistent with the current ones, hence relevant for semi-quantitative comparison: GWP and total primary energy demand. Table 4 below compares the 2005 results with the current results of acetone and phenol.

Table 4: Comparison of the present Eco-profile of Acetone and Phenol with their previous versions (2005)

Environmental Impact Categories	Acetone (2015)	Acetone (2005)	Difference	Phenol (2015)	Phenol (2005)	Difference
Gross primary energy from resources [MJ]	61,23	66,49	7%	67,02	66,49	1%
Global Warming Potential (GWP) [kg CO_2 eq.]	1,63	2,2	-25%	1,78	2,2	-19%

Although the previous model is unavailable for review, interpretations and explanations can be given based on the current results and thinkstep's experience.

The dominance analysis shows that both raw material inputs (main precursors and other chemicals) as well as energy supply have significant impact on the GWP and primary energy results. Therefore, the given changes in GWP and primary energy reflect the following technological improvement in the last 10 years in the production processes of the precursors as well as of the phenol and acetone themselves and are due to other factors that have an influence on the current results:

- Reduction of greenhouse gases emissions due to the energy generation with different energy carriers compared to year2005.
- Changes in the foreground and background system (updated emission factors; see Table 5):
  - Higher efficiency due to plants with higher production capacities
  - Improvements in energy management in the supply chain and the processing itself
  - Changes in the energy carrier mix used in the overall process chain
  - Stricter pollution and emissions control, such as exhaust air purification (POCP)
  - Changes in the electricity grid mix, in particular electricity from renewables becoming relevant, caused improvements in all impact categories.
- Methodological changes:
  - Compared with the 2005 version, the system boundaries now include the waste treatment of all wastes occurring in the process, so that only elementary flows cross the system boundary: this causes small changes in all impact categories. Please note that for the sake of comparability, waste arising is also reported on a foreground unit process level.
  - Allocation by energy content instead of mass

Table 5: Updated emission factors – cradle-to-gate - (based on GaBi database 2015, SP 28)

Electricity (EU-27 grid mix) ton CO_2 equiv./MWh	**Steam** ton CO_2 equiv./TJ enthalpy	**Steam** ton CO_2 equiv./TJ PFE
0,47	76,74	69,13
incl. exploration and supply of energy carriers	Steam production from natural gas (90% efficiency)	Steam production from natural gas (90% efficiency)

Information

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Programme Manager & Reviewer
DEKRA Assurance Services GmbH
This Environmental Product Declaration has been reviewed by DEKRA Assurance Services GmbH. It was approved according to the Product Category Rules PCR version 2.0 (2011-04) and ISO 14025:2006 [ISO 14025: 2006].
Registration number: PlasticsEurope 2016-002, validation expires on 30 September 2020 (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 www.plasticseurope.org.

Available data formats
The LCI data sets for phenol and acetone are available in the formats: GaBi, ecospold, ILCD, MS Excel® tables.

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

External Independent Review Summary

The subject of this critical review is the development of the Eco-profile for Phenol and Acetone. As mentioned in the report, the Eco-profiles for these two products did not encompass primary data collection from European manufacturers. Instead, an existing phenol and acetone dataset available in the GaBi database was used and revised based on additional information.

For that purpose, the available dataset information was shared with phenol and acetone producers who are part of the Cefic Phenol and Acetone Sector Group (PASG). Life cycle inventory data was checked against available primary information and adapted when considered appropriate. In addition, available emission data from the ETS rule book were considered (where possible) and again lead to further refinements of the dataset information.

The reviewer was involved in these activities right from the beginning and was able to provide advice in the resulting procedures. Several review meetings between PASG, the LCA practitioner (thinkstep AG) and the reviewer took place over a time period of over two years. The final Eco-profile report was reviewed by the reviewer as well as by PASG members involved in this project. All questions and recommendations were discussed with the LCA practitioner, and the report was adapted and revised accordingly.

The following information is of particular relevance for the above mentioned datasets and should be considered when using the Eco-profile for phenol and acetone:

- Instead of country-specific production conditions based on actual phenol/acetone manufacturing sites, EU-specific datasets for the background system have been used;
- Due to the above, no representativeness statement in the sense of a real European production average can be made;
- Due to the different procedure (as outlined above) for the development of the phenol and acetone Eco-profiles, a more concise project documentation was produced (compared to other Eco-profile projects);
- The possible allocation approaches for phenol and acetone production as well as the other by-products acetophenone and alpha-methylstyrene were discussed in detail. The chosen allocation method based on the energy content was considered most suitable and is justified in the report. Sensitivity analysis was carried out for the other possible allocation approaches.
- The report also contains a dominance analysis of phenol and acetone production showing the environmental hot-spots considering the cradle-to-gate lifecycle and provides a comparison of this Eco-profile with the previous version published in 2005.

For further details including the detailed results regarding the environmental performance of phenol and acetone, please refer to the report as well as the available datasets.

The LCA practitioner has demonstrated very good competence and experience, with a track record of LCA projects in the chemical and plastics industry. The critical review confirms that this Eco-profile is based on the rules set forth in the PlasticsEurope's Eco-profiles and Environmental Declarations – LCI Methodology and PCR for Uncompounded Polymer Resins and Reactive Polymer Precursors (PCR version 2.0, April 2011); the specific differences are outlined above. As a result, this dataset is assessed to be a reliable and high quality representation of phenol and acetone produced in Europe.

Name and affiliation of reviewer:

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

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