



Eco-profile

of three oxygenated solvent (groups):

n-Butanol, Butyl Glycol Ethers, Acetone

Nov 2021

1 SUMMARY

This Eco-profile report has been prepared according to the **Eco-profiles program and methodology –PlasticsEurope – V3.0 (2019)** with regards to the report layout, general structure and the chapters covered. As it is mentioned on several occasions later within chapter 2.10, the rules of the underlying LCA model are defined by and according to the **Guide for EF compliant data sets – V2.0 (2020)**

It provides average environmental performance data of a representative European market mix of each 1 kg of the following three oxygenated solvent (groups)

- n-Butanol
- Butyl Glycol Ethers
- Acetone

analysed from cradle to gate (from crude oil extraction to liquid solvents production at plant).

Please keep in mind that comparisons cannot be made on the level of the solvent 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.

It is intended to be used by the member companies, to support product-orientated environmental management; by users of solvents, 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.

The underlying developed, aggregated LCI datasets are compiled following the EF 3.0 standard [JRC 2020] and therefore can be used for the creation and modelling for future (product) environmental footprint (EF) studies/profiles according the official (P)EF guidance document [PEF GUIDE 2013].

1.1 META DATA

Data Owner	Oxygenated Solvent Producers Association (OSPA)
LCA Practitioner	Sphera Solutions GmbH
Programme Owner	PlasticsEurope
Reviewer	DEKRA Assurance Services GmbH, Angela Schindler

Number of plants included in data collection	3 (n-Butanol) 4 (Butyl Glycol Ethers) 6 (Acetone)
Representativeness	Butanol: about 100% of European production Butyl Glycol ethers: > 50% coverage in terms of European industry market Acetone: about 85% of European production
Reference year	2018 (Butanol / Butyl Glycol Ethers) 2019/2020 (Acetone)
Year of data collection and calculation	2021
Expected temporal validity	2026
Cut-offs	No significant cut-offs
Data Quality	Very good
Allocation method	Depending on product group

1.2 DESCRIPTION OF THE PRODUCT AND THE PRODUCTION PROCESS

This Eco-profile is for oxygenated solvents n-Butanol, Butyl Glycol Ethers, and Acetone. Oxygenated solvents are organic solvents, their molecules contain oxygen. These solvents are known for their significantly high rate of purity owing to the critical solvent refinement processes which eliminate excess water and particulate matter which occurs in various stages of production. Moreover, oxygenated solvents used industrially tend to have good solvency power and are wholly or partly miscible with water.

N-butanol is a primary alcohol (4-carbon, linear alcohol) that is butane in which a hydrogen of one of the methyl groups is substituted by a hydroxy group. Normal butanol is almost insoluble in water but is soluble in almost all organic solvents.

Butyl Glycol Ethers are organic compounds and butyl ethers of ethylene glycol. Like other glycol ethers, it has a bi-functional nature, containing both an ether and an alcohol group in the same molecule. It is fully miscible with water and a wide range of organic solvents. This excellent miscibility makes it a versatile solvent and coupling agent which offers excellent performance features in a wide range of applications.

Acetone is an organic compound, and it is the simplest and smallest ketone. Acetone is miscible with water and serves as an important organic solvent in its own right, in industry, home, and laboratory.

The reference flows, to which all data given in this Eco-profile refer, is 1 kg of n-butanol, 1 kg of (mixed) Butyl Glycol Ethers, and 1 kg of Acetone.

Production Process

N-Butanol

The process to produce n-butanol is Oxo synthesis process, also known as propylene hydroformylation to produce aldehydes, which are further hydrogenated to produce the butanol isomers.

Butyl Glycol Ethers

The dominant method to produce butyl glycol ethers is by reacting ethylene oxide with an alcohol such as normal butanol (n-butanol) within a catalyst. This process is called ethoxylation.

Acetone

Most acetone is produced utilizing Hock process. This study is only focused on acetone produced by the Hock process. The process starts with cumene being oxidized to form an intermediate compound called cumene hydroperoxide (CHP). The cumene hydroperoxide then goes through a cleavage reaction to form phenol and acetone.

Use Phase and End-of-Life Management

N-butanol can be used as a chemical intermediate to create other chemicals (e.g. Esters, n-butyl acetate and amino resins). Alternatively, it can be used as a solvent in the creation of consumer products. As a solvent it is applicable for paints, coatings, varnishes, fats, oils, waxes, rubber and plasticizers. Other uses include coating fabric in the textiles industry, as a cleaning or polishing agent, gasoline, brake fluid and in consumer products such as make-up, nail products, hygiene products and shaving products in the cosmetic industry. The main user end market of this product is the chemical, petrochemical, textiles, cleaning and cosmetics industries.

Butyl Glycol Ethers ether is most commonly used as a solvent and coalescing agent in water-based paints, coatings and inks where it improves the flow of the products as well as extending their drying time. It is also an efficient flow improver for urea, melamine and phenolic stoving finishes. Butyl Glycol Ethers is also favoured in many products due to its

mild odour. It acts as a solvent and coupling agent in many waxes, resins, oils and textile dyes, and is regularly used in many industrial, commercial and household cleaning products, where it offers good cleaning power as well as the odour typically associated with such products. It is an important starting material for a variety of syntheses, being one of the raw materials for the production of Butyl Glycol Ethers acetate and for the production of plasticizers by reaction with phthalic anhydride. It is also formulated into insecticides, herbicides, agricultural pesticides and cosmetic products, and is a component in hydraulic fluids and cutting and drilling oils.

Acetone is commonly used as a solvent to manufacture plastics and other industrial products. It may also be used to a limited extent in household products, including cosmetics and personal care products. Apart from its usage as a solvent, 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).

With regards to the End-of-Life (EoL) treatment of the solvents, of course, no general statements can be made as it is clearly depending on their specific application.

The following parameters for example do influence the consideration of potential EoL treatment options:

- Industrial or non- industrial/end-consumer applications
- Concentration of solvents/ degree of impurity
- Hazardousness/ toxicity of solvent / potential risks in solvent handling
- Price of solvent
- Environmental burden of solvent production
- Calorific value of solvent but also the related CO₂ emissions of its incineration – both being mainly influenced by the solvent specific carbon content
- Physical/ chemical properties (e.g. boiling range)

Only for industrial solvent uses a controlled treatment of solvent wastes can be assumed – apart from that, emission to air or municipal waste (water) treatment will be the common fate.

In an industrial context usually solvent recycling (either open or closed loop) via mostly rectification/ distillation and/or (ultimately) specific waste solvent incineration are the preferred options. The latter one can also be combined with energy recovery as organic solvents show a high calorific value.

1.3 DATA SOURCES AND ALLOCATION

The main data source was a data collection from European producers of n-Butanol, Butyl Glycol Ethers (with one company importing to Europe) and Acetone:

- N-Butanol: 3 plants, 2 different countries
- Butyl Glycol Ethers: 4 plants, 3 different countries
- Acetone: 6 plants, 5 different countries

For the solvents in scope of this study the following representativeness figures can be assumed:

- N - Butanol: about 100% of European production (based on EUROSTAT data)
- Butyl Glycol ethers: > 50% coverage in terms of European industry market (according to qualified expert judgement by OSPA)
- Acetone: about 85% of European production (based on EUROSTAT data)

The data for the upstream supply chain until the precursors, as well as all relevant background data such as energy and auxiliary material are taken from the GaBi 2020 LCI database [SPHERA 2020] and the available EF 3.0 compliant background datasets [EF DATABASE 2019], if applicable. Most of the background data used is publicly available and public documentation exists.

Generally, mass allocation has been applied as the method of choice in case of reported, valuable (and externally sold) by-products with an interdependent price ratio being below 20% (otherwise an economic allocation approach would have been followed, following the suggestion of [WBCSD 2014] and being in line with [JRC 2020]).

Regarding Acetone the allocation approach (allocation by energy content) of the existing Phenol/Acetone CEFIC Eco-profile was applied [CEFIC 2016]

1.4 ENVIRONMENTAL PERFORMANCE

The tables below show the environmental performance indicators associated with the production of 1 kg of each solvent (group):

1.4.1 Input Parameters

Indicator	Unit	Value			Impact method ref.
		Butanol	Butyl Glycol Ethers	Acetone	
Non-renewable energy resources ¹⁾					
• Fuel energy	MJ	42,81	44,07	33,83	-
• Feedstock energy	MJ	36,02	32,48	30,60	Gross calorific value
Renewable energy resources (biomass) ¹⁾					
• Fuel energy	MJ	1,47	2,32	1,35	-
• Feedstock energy	MJ	0,00	0,00	0,00	Gross calorific value-
Resource use					
• Minerals and Metals	kg Sb eq	3,00E-07	4,49E-07	2,40E-07	EF 3.0
• Energy Carriers	MJ	72,64	70,33	59,37	EF 3.0
Renewable materials (biomass)	kg	6,43E-14	1,36E-10	2,43E-11	-
Water scarcity	m ³ world eq	4,89E-02	1,65E-01	2,00E-01	EF 3.0
¹⁾ Calculated as upper heating value (UHV)					

1.4.2 Output Parameters

Indicator	Unit	Value			Impact method ref.
		Butanol	Butyl Glycol Ethers	Acetone	
Climate change, total	kg CO ₂ eq.	2,48	2,45	1,91	EF 3.0
Ozone depletion	kg CFC-11 eq.	2,55E-11	2,58E-11	7,62E-12	EF 3.0
Acidification	Mole of H ⁺ eq	3,75E-03	4,57E-03	2,73E-03	EF 3.0
Photochemical ozone formation	kg NMVOC eq	2,91E-03	5,90E-03	2,84E-03	EF 3.0
Eutrophication, freshwater	kg P eq	2,04E-06	8,63E-06	3,34E-06	EF 3.0
Respiratory Inorganics	Disease incidences	2,62E-08	5,81E-08	2,26E-08	EF 3.0
Waste					

• Non-hazardous	kg	0,98	1,28	0,37	-
• Hazardous	kg	3,94E-04	7,70E-04	2,01E-04	-

Please refer to chapter 4 for a complete overview of all EF 3.0 indicator results of the products in scope.

1.5 PROGRAMME OWNER

PlasticsEurope

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1.6 DATA OWNER

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1.7 LCA PRACTITIONER

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1.8 REVIEWER

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2 ECO-PROFILE REPORT

2.1 FUNCTIONAL UNIT AND DECLARED UNIT

n-Butanol: 1 kg of primary n-Butanol »at gate« (production site output) representing the average of the participating companies

Butyl Glycol Ethers: 1 kg of primary, mixed (company specific mixes/shares of distinct) Butyl Glycol Ethers »at gate« (production site output) representing the average of the participating companies

Acetone: 1 kg of primary Acetone »at gate« (production site output) representing the average of the participating companies

2.2 PRODUCT DESCRIPTION

N-butanol

- IUPAC name : Butan-1-ol
- CAS numbers covered in this study: 71-36-3
- chemical formula: $C_4H_{10}O$
- gross calorific value: 36.02 MJ/kg

Butyl Glycol Ethers

- IUPAC names:
 - 2-Butoxyethan-1-ol,
 - 2-(2-Butoxyethoxy)ethanol
 - 2-[2-(2-Hydroxyethoxy)ethoxy]ethanol
- CAS numbers covered in this study: 111-76-2, 112-34-5, 112-27-6
- chemical formulas: $C_6H_{14}O_2$, $C_8H_{18}O_3$, $C_6H_{14}O_4$
- gross calorific value: approx¹. 32,5 MJ/kg

¹ Value taken from GaBi database, using 2-Butoxyethan-1-ol as reference

Acetone

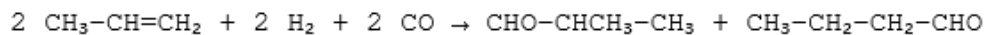
- IUPAC name: Propan-2-one
- CAS numbers covered in this study: 67-64-1
- chemical formula: C₃H₆O
- gross calorific value: 30.60 MJ/kg

2.3 MANUFACTURING DESCRIPTION

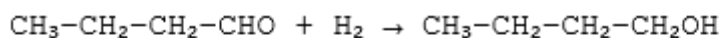
n-butanol

N-butanol is produced by the Oxo synthesis process, also known as propylene hydroformylation. This low-pressure liquid-phase process combines liquid-phase propylene and aldehydes (a 1:1 mixture of hydrogen and carbon monoxide) in the presence of modified Rhodium catalysts to produce aldehydes, which are further hydrogenated to produce the butanol isomers. This process is typically optimized for production of n-butanol, with yields of up to 98% n-butanol.

Step 1: Preparation of Butanal:



Step 2: Hydrogenation of Butanal to n-Butanol:

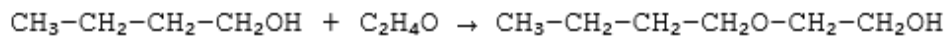


Butyl Glycol Ethers

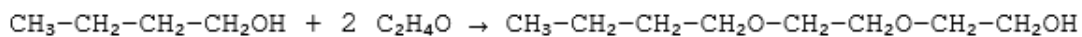
Ethylene glycol butyl ether (EGBE), also called 2-Butoxyethanol, is a colourless liquid and one of the simplest glycol monoalkyl ethers. Ethylene glycol mono alkyl ethers are not manufactured as pure compounds but must be separated from the diethers and higher glycols. There are two common methods of producing ethylene glycol butyl ether: reaction of ethylene oxide with anhydrous butyl alcohol in the presence of a catalyst and direct alkylation of ethylene chlorohydrin or ethylene glycol using sodium hydroxide and an alkylating agent such as dibutyl sulfate. By far the dominant method of ethylene glycol butyl ether production

is treatment of butyl alcohol with ethylene oxide. Depending on the molar ratios of the raw materials (the ratio of ethylene oxide to n-butanol greater than one initiates the production of di- and tri-ethylene glycol monoethers along with the EGBE), varying amounts the monoethylene, diethylene, triethylene and higher glycol ethers are obtained. Thus, the further treatment is the separation and purification by fractional distillation to obtain the desired product.

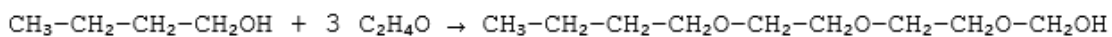
Preparation of EGBE:



Preparation of diethylene glycol butyl ether (DEGBE):



Preparation of triethylene glycol butyl ether (TEGBE):

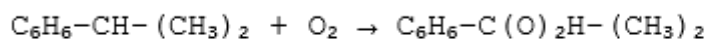


Acetone

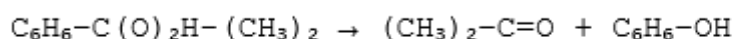
Acetone is produced utilizing Hock process as described below:

- Cumene (i-propyl benzene) is oxidized by exposure to air to temporarily produce cumene hydroperoxide:
- The cumene hydroperoxide is simply cleaved at the top of the benzene ring using an acidic catalyst to produce the two usable products of phenol and acetone.
- The catalyst is extracted, and the phenol/acetone mixture is fractionated and purified.

Step 1: Preparation of cumene hydroperoxide:



Step 2: Preparation of Acetone and Phenol:



2.4 PRODUCER DESCRIPTION

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

Company	Address	Contribution to		
		Butanol	Butyl Glycol Ethers	Acetone
BASF	BASF SE Carl-Bosch-Strasse 38 67056 Ludwigshafen Germany	X	X	
CEPSA	Cepsa Química S. A. Polígono Industrial Nuevo Puerto, s/n, 21810 Palos de la Frontera, Huelva Spain			X
DOMO	Domo Caproleuna GmbH Am Haupttor Bau 3101 06237 Leuna Germany			X
Eastman	Eastman Chemical Company 200 S Wilcox Dr Kingsport, TN USA		X	
INEOS Oxide	INEOS Oxide Avenue des Uttins 3 Rolle 1180 Switzerland	X	X	
INEOS Phenol	INEOS Europe AG – Phenol division Avenue des Uttins 3 Rolle 1180 Switzerland			X
OQ	OQ Chemicals GmbH Rheinpromenade 4a 40789 Monheim am Rhein Germany	X		
Sasol	Sasol Germany GmbH Anckelmannsplatz 1 20537 Hamburg Germany		X	

Seqens Solvents and Phenol Specialities	SEQENS SAS 21, chemin de la sauvegarde 21 Ecully Parc - CS 33167 69134 Ecully Cedex France			X
Versalis	Versalis S.p.A. Piazza Boldrini 1 San Donato Milanese Italy			X

2.5 SYSTEM BOUNDARIES

PlasticsEurope Eco-profiles refer to the production of solvents as a cradle-to-gate system (see Figure 1 for N-butanol, Figure 2 for Butyl Glycol Ethers, and Figure 3 for Acetone).

Although for some companies also the reported primary data of pre-cursors production has been considered (and modelled), the diagrams show the common minimum foreground system.

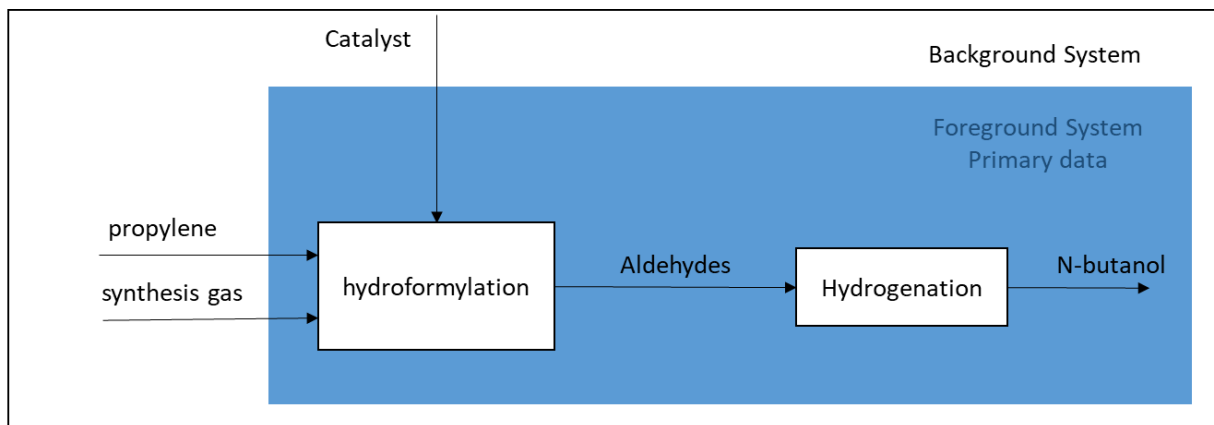


Figure 1: Cradle-to-gate system boundaries (N-butanol)

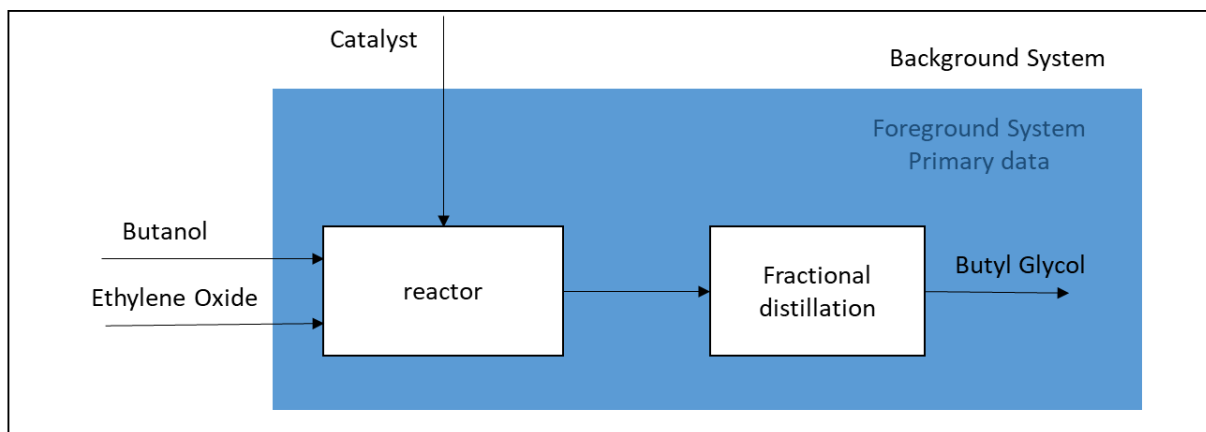


Figure 2: Cradle-to-gate system boundaries (Butyl Glycol Ethers)

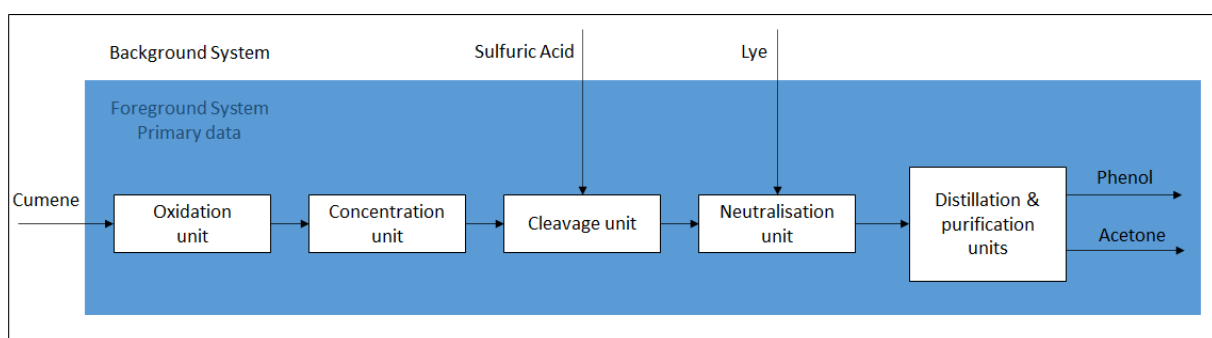


Figure 3: Cradle-to-gate system boundaries (Acetone)

2.6 TECHNOLOGICAL REFERENCE

The production processes were modelled using specific values from primary data collection at site, representing the specific technology for the data reporting companies. The LCI data represent technology in use in the defined production region employed by participating producers. The considered participants cover at least 50% of the European industry market in the reference years mentioned above:

- N - Butanol: about 100% of European production (based on EUROSTAT data)
- Butyl Glycol ethers: > 50% coverage in terms of European industry market (according to qualified expert judgement by OSPA)
- Acetone: about 85% of European production (based on EUROSTAT data)

Primary data were used for all foreground processes (under operational control) complemented with secondary data from background processes (under indirect management control).

2.7 TEMPORAL REFERENCE

The LCI data for production was collected as 12-month averages representing the year 2018/2020, to compensate for seasonal influence of data.

Background data have reference year from 2019 (Sphera data), and 2012/2015 regarding the EF 3.0 datasets.

The average datasets are considered to be valid until substantial technological changes in the production chain occur. Having the latest technology development in mind, the companies participating in this Eco-profile define as temporal reference: the overall reference year for this Eco-profile is 2018 with a recommended temporal validity until 2026.

2.8 GEOGRAPHICAL REFERENCE

Primary production data have been reported from production sites within EU (with one company producing and importing Butyl Glycol Ethers from the US). Fuel and energy inputs in the system reflect whenever applicable and possible, site specific conditions – otherwise average European conditions were applied – to reflect representative situations. Therefore, the study results are intended to be applicable within EU boundaries and in order to be applied in other regions adjustments might be required.

2.9 CUT-OFF RULES

In the foreground processes all reported flows were considered, trying to avoid any cut-off of material and energy flows.

According to the GaBi 2020 LCI database [SPHERA 2020], and [EF DATABASE 2019] used in the background processes, at least 95% of mass and energy of the input and output flows were covered and 98% of their environmental relevance (according to expert judgment) was considered, hence an influence of cut-offs less than 1% on the total is expected

2.10 DATA QUALITY REQUIREMENTS

Data Sources

Eco-profiles developed by ESIG (OSPA) use average data representative of the respective foreground production process, both in terms of technology and market share. The primary data are derived from site specific information for processes under operational control supplied by the participating member companies of ESIG (see 2.4).

The data for the upstream supply chain is taken from the GaBi 2020 LCI database [SPHERA 2020] of the software system GaBi 10 and the officially available EF 3.0 datasets [EF DATABASE 2019], if applicable².

The same applies for background data such as energy and auxiliaries. Most of the background data used is publicly available and public documentation exists.

Relevance

Regarding the goal and scope of this Eco-profile, the collected primary data of foreground processes are of high relevance, i.e. data was sourced from the most important solvents producers in Europe in order to generate a European industry average. The environmental contributions of each process to the overall LCI results are included in the Chapter 'Dominance Analysis'.

Representativeness

The considered participants covered at least 50% of the European industry market (2018) regarding the solvents in scope of this assessment. The selected background data can be regarded as representative for the intended purpose, as it is average data

Consistency

To ensure consistency only primary data of the same level of detail and background data from the GaBi 2020 LCI database [SPHERA 2020] were used. While building up the model, cross-checks concerning the plausibility of mass and energy flows were continuously conducted. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system.

² Due to the project goal of developing EF 3.0 compliant datasets, the background datasets need to be taken from the current version of the EF Reference Package (v3) (with the reference year 2012 for energy datasets).

Reliability

Data reliability ranges from measured to estimated data. Data of foreground processes provided directly by producers were predominantly measured. Data of relevant background processes were measured at several sites or determined by literature data or estimated for some flows, which have been reviewed and checked for its quality.

Completeness

Primary data used for the gate-to-gate production of the solvents in scope of this assessment all related flows in accordance with the cut off criteria. In this way all relevant flows were quantified, and data is considered complete.

Precision and Accuracy

As the relevant foreground data is primary data or modelled based on primary information sources of the owner of the technology, better precision is not reachable within this goal and scope. All background data is consistently GaBi professional data with related public documentation.

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 GaBi 10 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 in a certain confidence range.

Data Validation

The data on production collected from the project partners and the data providing companies was validated in an iterative process several times. The collected data was validated using existing data from published sources or expert knowledge.

The background information from the GaBi 2020 LCI database [SPHERA 2020] is updated regularly and validated and benchmarked daily by its various users worldwide.

Life Cycle Model

The study has been performed with the LCA software GaBi 10. The associated database integrates ISO 14040/44 requirements. LCA modelling has been carried out following the rules of EF 3.0 compliant dataset modelling [JRC 2020]

Due to confidentiality reasons details on software modelling and methods used cannot be shown here. However, in principle the model can be reviewed in detail if the data owners agree. The calculation follows the vertical calculation methodology, i.e. that the averaging is done after modelling the specific processes.

2.11 CALCULATION RULES

Vertical Averaging

When modelling and calculating average Eco-profiles from the collected individual LCI datasets, vertical averages were calculated (Figure 4).

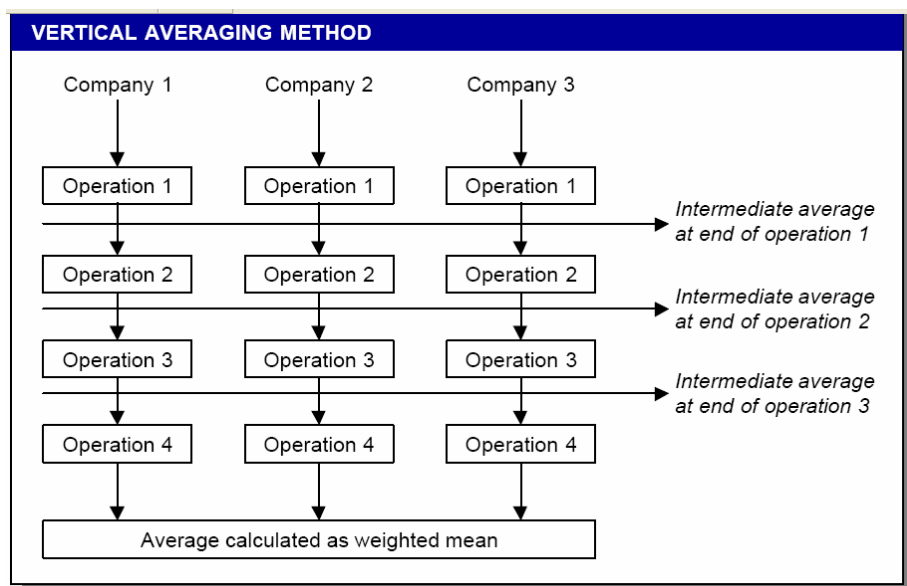


Figure 4: Vertical Averaging (source: Eco-profile of high-volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)

Allocation Rules

Production processes in chemical and plastics industry are usually multi-functional systems, i.e. they have not one, but several valuable product and co-product outputs. Wherever possible, allocation should be avoided by expanding the system to include the additional functions related to the co-products. Often, however, avoiding allocation is not feasible in technical reality, as alternative stand-alone processes are not existing, or alternative

technologies show completely different technical performance and product quality output or no clear dominant route is available for credit generation. 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.

Generally, mass allocation has been applied as the method of choice in case of reported, valuable (and externally sold) by-products with an interdependent price ratio being below 20% (otherwise an economic allocation approach would have been followed, following the suggestion of [WBCSD 2014] and being in line with [JRC 2020]).

Regarding Acetone the allocation approach (allocation by energy content) of the existing Phenol/Acetone CEFIC Eco-profile was applied [CEFIC 2016]

In the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [SPHERA 2020]. The chosen allocation in refinery is based on several sensitivity analyses, which was accompanied by petrochemical experts. The relevance and influence of possible other allocation keys in this context is small. In steam cracking, allocation according to net calorific value is applied. Relevance of other allocation rules (mass) is below 2 %.

2.12 LIFE CYCLE INVENTORY (LCI) RESULTS

Delivery and Formats of LCI Dataset

This eco-profile comprises

- One EF 3.0 compliant dataset per average solvent in ILCD/EF 3.0 format (<https://eplca.jrc.ec.europa.eu/LCDN/developer.xhtml>) according to the last version at the date of publication of the Eco-profile and including the reviewer (internal and external) input.
- This report in pdf format.

Energy Demand

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 **energy content in the solvents** indicates a measure of the share of primary energy incorporated in the product, and hence a recovery potential (system output), quantified as the gross calorific value (UHV).

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

Table 1 Primary energy demand (system boundary level) per 1kg n-Butanol

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	36,02
Process energy (quantified as difference between primary energy demand and energy content of solvent)	44,28
Total primary energy demand	80,30

Table 2 Primary energy demand (system boundary level) per 1kg Butyl Glycol Ethers

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	32,48
Process energy (quantified as difference between primary energy demand and energy content of solvent)	46,39
Total primary energy demand	78,87

Table 3 Primary energy demand (system boundary level) per 1kg Acetone

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	30,60
Process energy (quantified as difference between primary energy demand and energy content of solvent)	35,18
Total primary energy demand	65,78

Water cradle to gate Use and Consumption

The cradle-to-gate³ blue water **use** accounts for

- n-Butanol: 727,9 kg
- Butyl Glycol Ethers: 1150,4 kg
- Acetone: 458,5 kg

The corresponding blue water **consumption** in the same system boundary shows as

- n-Butanol: 6,2 kg
- Butyl Glycol Ethers: 9,7 kg
- Acetone: 6,5 kg

Water foreground (gate to gate) Use and Consumption

The following tables show the weighted average values for water use of the solvents production process (gate-to-gate level). For each of the typical water applications the water sources are shown.

Table 4 Water use and source per 1kg of n-Butanol

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0,00	0,00	0,00	0,00	0,00
Deionized / Softened	0,05	0,06	0,90	0,00	1,01
Untreated (from river/lake)	0,00	21,34	0,00	0,00	21,34
Untreated (from sea)	0,00	0,00	0,00	0,00	0,00
Relooped	0,00	0,00	0,20	0,00	0,20
Totals	0,05	21,40	1,10	0,00	22,55

³ This includes water use in the total upstream supply chain

Table 5 Water use and source per 1kg of Butyl Glycol Ethers

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0,06	0,01	0,00	0,00	0,07
Deionized / Softened	0,03	0,03	1,85	0,00	1,92
Untreated (from river/lake)	0,00	7,71	0,00	0,00	7,71
Untreated (from sea)	0,00	28,61	0,00	0,00	28,61
Relooped	0,00	27,21	0,42	0,00	27,63
Totals	0,09	63,57	2,27	0,00	65,93

Table 6 Water use and source per 1kg of Acetone

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0,24	37,70	0,02	0,00	37,96
Deionized / Softened	0,72	0,09	1,29	0,01	2,12
Untreated (from river/lake)	0,00	3,94	0,00	0,00	3,94
Untreated (from sea)	0,00	0,00	0,00	0,00	0,00
Relooped	0,00	36,51	0,16	0,00	36,67
Totals	0,97	78,24	1,48	0,01	80,69

The following tables show the further handling/processing of the water output of the production processes of the solvents:

Table 7 Treatment of Water Output per 1kg of n-Butanol

Treatment	Water Output [kg]
To WWTP	0,13
Untreated (to river/lake)	20,86
Untreated (to sea)	0,07
Relooped	0,39
Water leaving with products	0,00
Water Vapour	1,10
Formed in reaction (to WWTP)	0,01
Totals	22,56

Table 8 Treatment of Water Output per 1kg of Butyl Glycol Ethers

Treatment	Water Output [kg]
To WWTP	0,40
Untreated (to river/lake)	7,41
Untreated (to sea)	28,65
Relooped	28,31
Water leaving with products	0,00
Water Vapour	1,16
Formed in reaction (to WWTP)	0,01
Totals	65,93

Table 9 Treatment of Water Output per 1kg of Acetone

Treatment	Water Output [kg]
To WWTP	1,28
Untreated (to river/lake)	2,98
Untreated (to sea)	0,25
Re looped	74,54
Water leaving with products	0,00
Water Vapour	1,63
Formed in reaction (to WWTP)	0,00
Totals	80,69

Based on the water use and output figures above the **water consumption** can be calculated as:

Consumption = (water vapour + water lost to the sea) – (water generated by using water containing raw materials + water generated by the reaction + seawater used)

- n-Butanol = 1,16 kg
- Butyl Glycol Ethers = 1,20 kg
- Acetone = 1,87 kg

Contrasting the GWP result for Acetone calculated within this study with the carbon footprint published in the CEFIC Eco-profile [CEFIC 2016] shows the following difference when applying the same impact assessment methodology (CML):

1,85 kg CO₂ eq (OSPA, 2021) vs 1,64 kg CO₂ eq (CEFIC, 2016)

The following reasons influence those results and explain the different outcome:

- The result presented in this study is based on (measured) primary data, while the CEFIC study was built on literature and other secondary data
- The background datasets for raw materials, energy and auxiliaries used in this study have been selected regional specific, while in the CEFIC report EU average datasets have been used
- As the modelling applied in this study followed the guide on creating EF 3.0 compliant datasets specific calculation and modelling principles were followed (such as adding infrastructure/capital goods, CFF formula to account for secondary fuel inputs and waste for recovery)

3 REVIEW

3.1 EXTERNAL INDEPENDENT REVIEW SUMMARY



Critical Review Statement

Eco-profile of three oxygenated solvent (groups):
n-Butanol, Butyl Glycol Ethers, Acetone

Commissioned by:	Oxygenated Solvent Producers Association (OSPA)
Version:	Eco-profile, October 2021
Prepared by:	Yannick Bernard, Sphera Solutions GmbH
Reviewed by:	Angela Schindler, DEKRA Assurance Services GmbH
References:	<ul style="list-style-type: none">▪ ISO 14040 (2006): Environmental Management – Life Cycle Assessment – Principles and Framework▪ ISO 14044 (2006): Environmental Management – Life Cycle Assessment – Requirements and Guidelines▪ Eco-profiles program and methodology – PlasticsEurope, v3.0 (2019)

External independent review

This Eco-profile covers the declaration of the environmental performance of three oxygenated solvent groups:

- n-Butanol
- Butyl Glycol Ethers
- Acetone

The Eco-profile document was sent and reviewed in September/October 2021.

The compliance of the documents was reviewed according to the current requirements of the Eco-profiles program and methodology, version 3.0 (Oct 2019) of PlasticsEurope. Besides, the substantial intention of this Eco-profile is the generation of life cycle inventories for the above mentioned substances, according to the Guide for EF compliant data sets, version 2.0 (2020), to be used as background data for environmental footprint studies, according to the European Commission's PEF Guide (2013).

Thus, the software modelling, applied data sets and the assessment follows the published rules of the European Platform on Life Cycle Assessment (EPLCA) and the Joint Research Centre (JRC).

The review process covered the annotation of the Eco-profile by commenting the submitted Eco-profile report. In an extensive webmeeting the confidential data collection and the software model was shown to the reviewer; the comments on the documents were discussed and questions clarified by explanations of the LCA practitioner.

Main producers have taken part in this study. Regionalization of material and energy flows has been implemented as far as datasets were available. Thus, the Eco-profile can be seen as representative for the European market.

From the life cycle assessment perspective, the processing of the three declared substances and/or the distribution channel is very similar and thus are combined in one Eco-profile.

The practitioner followed the recommendation of the reviewer to supplement the manufacturing description by chemical notation, which enables experts an unambiguous understanding of the included processing steps.

Due to the intention to generate a PEF-conform LCI, the software model integrates only official background data of the EF 3.0 database of the European Commission, as far as they are available, supplemented with datasets of the current GaBi database. As the EF 3.0 database was generated as a static database during the PEF pilot project, the applied background data are still valid, but refer to an older technological status, mainly 2012 – 2015. This compromise is necessary to meet all given requirements. This is valid especially in regard to the dynamically changing electricity grid mixes; in the current study the contribution of electricity can be seen as a minor contributing factor.

In this context it is worth to mention, that the PEF guide prescribes the avoided burden approach for secondary input materials as well as the circular footprint formula for EoL of production residues. These methodological approaches are controversial and thus create inconsistencies in currently generated life cycle inventories published not completely following all rules of the PEF guide.

The currently updated background data of the cracking process is controversially discussed in respect to scientific resilience. Thus, the present study integrates the back-ground data of EF 3.0/ GaBi database.

The applied allocations are traceable. The justification of the applied criteria has been discussed in the review process. Further sensitivity analyses were not necessary to be considered.

All further editorial recommendations of the reviewer were implemented by the practitioner.

Eco-profiles typically cover the system boundaries cradle-to-gate. During the review discussion an additional aspect in respect to a potential end-of-life scenario has been integrated. Although in this case the input materials comprise only fossil based materials, the indication of the consideration of the C-content per specific product (group) is essential for the correct application of the life cycle inventory in follow-up product Carbon Footprint calculations.

The software model applied has undergone a Sphera internal quality check to avoid mis-takes of data transfer. Overall, the project is carried out very thoroughly.

For future optimisation and improvement of the data, the participating companies are called to monitor and report also their water demand and sewage amounts in a more detailed manner. In respect to follow-up effects of global warming the topic water need to be looked at with higher awareness.

The structure and description of the Eco-profile is clear and transparent, thus displaying a reliable source of information.

Salem, 26.10.2021


Angela Schindler
Accredited Reviewer on behalf of DEKRA Assurance Services GmbH

3.2 REVIEWER CONTACT DETAILS

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4 EF 3.0 INDICATOR RESULTS

The following table shows the full list of EF 3.0 indicator results for each of the product groups :

Table 13 : EF 3.0 indicator results for selected OSPA solvents

Indicator	Unit	n-Butanol	Butyl Glycol Ethers	Acetone
Climate change, total	kg CO ₂ eq.	2,48	2,45	1,91
Climate Change, biogenic	kg CO ₂ eq.	9,68E-03	1,04E-02	1,06E-02
Climate Change, fossil	kg CO ₂ eq.	2,47	2,44	1,90
Climate Change, land use and land use change	kg CO ₂ eq.	5,14E-04	1,53E-03	4,47E-04
Ozone depletion	kg CFC-11 eq.	2,55E-11	2,58E-11	7,62E-12
Acidification	Mole of H+ eq	3,75E-03	4,57E-03	2,73E-03
Photochemical ozone formation	kg NMVOC eq	2,91E-03	5,90E-03	2,84E-03
Eutrophication, freshwater	kg P eq	2,04E-06	8,63E-06	3,34E-06
Eutrophication, marine	kg N eq.	7,67E-04	1,45E-03	7,77E-04
Eutrophication, terrestrial	Mole of N eq.	8,22E-03	1,55E-02	8,33E-03
Respiratory Inorganics	Disease incidences	2,62E-08	5,81E-08	2,26E-08
Ionising radiation, human health	kBq U235 eq.	0,07	0,14	0,03
Human toxicity, cancer – total	CTUh	8,79E-10	9,62E-10	7,27E-10
Human toxicity, cancer inorganics	CTUh	6,59E-20	1,82E-19	2,71E-20
Human toxicity, cancer metals	CTUh	7,62E-10	7,48E-10	6,02E-10
Human toxicity, cancer organics	CTUh	1,16E-10	2,13E-10	1,24E-10
Human toxicity, non-cancer – total	CTUh	3,93E-08	3,72E-08	2,98E-08
Human toxicity, non-cancer inorganics	CTUh	7,01E-09	6,90E-09	5,75E-09
Human toxicity, non-cancer metals	CTUh	3,23E-08	3,02E-08	2,40E-08
Human toxicity, non-cancer organics	CTUh	3,98E-10	5,06E-10	3,68E-10

Ecotoxicity, freshwater – total	CTUe	3,81E+01	3,36E+01	3,09E+01
Ecotoxicity, freshwater inorganics	CTUe	3,66E+01	3,06E+01	2,98E+01
Ecotoxicity, freshwater metals	CTUe	1,23E+00	2,71E+00	8,56E-01
Ecotoxicity, freshwater organics	CTUe	2,52E-01	3,35E-01	2,38E-01
Land Use	Pt	1,28E+00	2,98E+00	1,03E+00
Resource use, energy carriers	MJ	72,64	70,33	59,37
Resource use, minerals and metals	kg Sb eq.	3,00E-07	4,49E-07	2,40E-07
Water scarcity	m ³ world equiv.	4,89E-02	1,65E-01	2,00E-01

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