EUROPEAN SOLVENTS INDUSTRY GROUP

Eco-profile

of three hydrocarbon solvent groups:

Cat. 3 solvents, Cat. 6 solvents, Cat. 8 solvents

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)**

This provides average environmental performance data of a representative European market mix of each 1 kg of the following three hydrocarbon solvent categories[1]

- Cat. 3 solvents
- Cat. 6 solvents
- Cat. 8 solvents

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] For more information on the categories please refer to HSPA Naming Convention: https://www.esig.org/wp-content/uploads/2019/12/201910_HSPA-naming-convention-_October-2019.pdf

1.1 META DATA

Data Owner	Hydrocarbon Solvent Producers Association (HSPA)
LCA Practitioner	Sphera Solutions GmbH
Programme Owner	PlasticsEurope
Reviewer	DEKRA Assurance Services GmbH, Angela Schindler
Number of plants included in data collection	3 (Cat. 3 solvents) 4 (Cat. 6 solvents) 3 (Cat. 8 solvents)
Representativeness	> 50% of total volume produced coverage in terms of European industry market
Reference year	2018
Year of data collection and calculation	2021
Expected temporal validity	2026
Cut-offs	No significant cut-offs
Data Quality	Very good
Allocation method	Mass allocation

1.2 DESCRIPTION OF THE PRODUCT AND THE PRODUCTION PROCESS

This Eco-profile is for hydrocarbon solvents categories 3,6, and 8 (contained substances are listed in sec. 2.2). Hydrocarbon solvent substances are commonly derived from petroleum feedstocks and contain one or more hydrocarbon classes (e.g. linear, branched or cyclic alkanes and aromatics).

The difference between the types of hydrocarbon solvents is mainly due to their different hydrocarbon classes and their carbon chain length distribution. The carbon chain length distribution depends on the targeted distillation range of the final product. The hydrocarbon solvent carbon chain lengths are typically narrow cuts of hydrocarbon lengths over C5 and below C20.

The reference flows, to which all data given in this Eco-profile refer, is 1 kg of Cat. 3 solvents, 1 kg of Cat. 6 solvents, and 1 kg of Cat. 8 solvents.

Production Process

The major process for transforming petroleum feedstocks into hydrocarbon solvent substances is a combination of various process steps that may include distillation of the feedstock, hydrodesulphurization, mild or heavy hydrogenation, and finally a distillation and a stripping of light components.

Use Phase and End-of-Life Management

Hydrocarbon solvents are petroleum derivatives used for cleaning and or dissolving substances, and are used in a variety of industrial and consumer products. Some examples of hydrocarbon solvents are white spirit and hexane.

White spirit is used in paints, coatings, waxes, varnishes, adhesives, printing inks and liquid photocopier toners. In industry it is also used as a solvent for, cleaning, degreasing and substance extraction. In households, white spirit is commonly used to clean paint brushes or thin paint.

Hexane solvents are mainly used to extract edible oils from seed and vegetable crops (e.g., soybeans, peanuts, corn). Commercial grades of hexane are used as solvents for glues (rubber cement, adhesives), varnishes, and inks. It is also used as a cleaning agent (degreaser) in the printing industry.

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 CO_2 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 applications 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 Cat. 3, Cat. 6 and Cat. 8 solvents:

- Cat. 3: 3 plants, 3 different countries
- Cat. 6: 4 plants, 4 different countries
- Cat. 8: 3 plants, 3 different countries

For all solvents in scope of this study at least 50% of the European market (EU-28) in 2018 are covered - according to qualified expert judgement by HSPA.

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.

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]).

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.**
		Cat. 3	**Cat. 6**	**Cat. 8**	
Non-renewable energy resources[1)]					
• Fuel energy	MJ	7,29	10,24	9,61	-
• Feedstock energy	MJ	47,30	48,10	47,30	Gross calorific value
Renewable energy resources (biomass)[1)]					
• Fuel energy	MJ	0,13	0,24	0,17	-
• Feedstock energy	MJ	0,00	0,00	0,00	Gross calorific value-
Resource use					
• Minerals and Metals	kg Sb eq	1,03E-07	1,14E-07	1,10E-07	EF 3.0
• Energy Carriers	MJ	50,86	54,26	52,94	EF 3.0
Renewable materials (biomass)	kg	2,36E-14	2,62E-14	1,50E-14	-
Water scarcity	m^3 world eq	2,39E-03	1,52E-02	1,02E-02	EF 3.0
[1)] Calculated as upper heating value (UHV)					

1.4.2 Output Parameters

Indicator	**Unit**	**Value**			**Impact method ref.**
		Cat. 3	**Cat. 6**	**Cat. 8**	
Climate change, total	kg CO_2 eq.	0,53	0,84	0,67	EF 3.0
Ozone depletion	kg CFC-11 eq.	9,79E-13	1,46E-11	1,04E-11	EF 3.0
Acidification	Mole of H+ eq	2,80E-03	3,54E-03	2,94E-03	EF 3.0
Photochemical ozone formation	kg NMVOC eq	2,09E-03	2,47E-03	2,07E-03	EF 3.0
Eutrophication, freshwater	kg P eq	1,03E-06	9,54E-07	6,15E-07	EF 3.0
Respiratory Inorganics	Disease incidences	1,73E-08	2,18E-08	1,83E-08	EF 3.0
Waste					
• Non-hazardous	kg	0,01	0,03	0,01	-

• Hazardous	kg	5,13E-05	1,35E-04	9,54E-05	-

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

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2 ECO-PROFILE REPORT

2.1 FUNCTIONAL UNIT AND DECLARED UNIT

Cat. 3 solvents: 1 kg of primary Cat. 3 solvents »at gate« (production site output) representing the average of the participating companies

Cat. 6 solvents: 1 kg of primary Cat. 6 solvents »at gate« (production site output) representing the average of the participating companies

Cat. 8 solvents: 1 kg of primary Cat. 8 solvents »at gate« (production site output) representing the average of the participating companies

2.2 PRODUCT DESCRIPTION

As not every producer covered in this study is offering each of the distinct substances mentioned below in this chapter (which have been grouped and categorized following a naming convention for REACH registration [HSPA]), the participants have collected data for one or several representative substances (in terms of production volume and/or economic importance) falling under these categories.

Chapter 2.3 describes the manufacturing of “white spirits” (cat.3) and “de-aromatized white spirits” (cat. 8) - which are both mixtures of several substances of category specific substances itself - and hexane as representative for cat. 6, as these have been mostly selected as representative products by the participating companies.

It can be observed though that the production process and the herewith related environmental burden for all distinct products falling under a specific solvents’ category is considered to be very similar.

The following sub-chapters show all current products contained in the defined categories together with their EC number. For an overview of the relationship CAS to EC number, please consult [ESIG 2018]

Category 3 solvents: C9-14 Aliphatics (2-25% Aromatics)

The substances in the C_9-C_{14} Aliphatic [2-25% aromatic] Hydrocarbon Solvents Category contain >99% hydrocarbons. Category members are described as UVCBs (Unknown or Variable Composition, Complex Reaction Products and Biological Materials) because they are composed of a defined, progressive carbon number range that includes various types of hydrocarbons: aliphatic molecules (linear, branched, and cyclic) and aromatic molecules (generally one-ring alkylbenzenes), predominantly in the C_9 to C_{14} range. Benzene and sulfur content of category members is extremely low, typically <10 ppm with some substances identified as having <100 ppm, because these compounds are intentionally removed.

The substances and their identifiers are listed below:

HSPA Substance Name	CAS Number	EC Number
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	n.a.	927-344-2
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	n.a.	919-164-8
Hydrocarbons, C9-C12, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	n.a.	919-446-0
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	n.a.	925-653-7
Hydrocarbons, C12-C16, n-alkanes, isoalkanes, cyclics, aromatics (2-25%)	n.a.	920-008-6

As representative gross calorific value of 47,3 MJ/kg per solvent is approximated[2].

Category 6 solvents: C6 Aliphatics

C6 aliphatic solvents are complex and variable combinations of aliphatic constituents, primarily n-hexane, iso-hexane isomers, cyclohexane, and methyl cyclopentane in varying amounts, and boiling in the range of approximately 55–85°C with most of the category members described as UVCBs. The C6 aliphatic solvents are colorless liquids at room temperature, with slightly disagreeable odors. The benzene and sulfur contents of hydrocarbon solvents in the C6 aliphatic hydrocarbon category are low, with benzene levels typically <1 ppm.

The substances and their identifiers are listed below:

HSPA Substance Name	CAS Number	EC Number
n-Hexane	110-54-3	203-777-6
Hydrocarbons, C6, isoalkanes, <5% n-Hexane	n.a.	931-254-9

[2] Value taken from GaBi database, using Naphtha as reference

Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	n.a.	925-292-5
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, <5% n-Hexane	n.a.	922-114-8
Hydrocarbons, C6-C7, isoalkanes, cyclics, <5% n-Hexane	n.a.	926-605-8
Hydrocarbons, C5-C7, n-alkanes, isoalkanes, n-hexane rich	n.a.	930-397-4
2-Methyl-pentane	43133-95-5	639-864-4
2,2 Dimethyl-butane	75-83-2	200-906-8
2,3 Dimethyl-butane	79-29-8	201-193-6

As representative gross calorific value of 48,1 MJ/kg per solvent is approximated[3].

Category 8 solvents: C9-14 Aliphatics (<=2% aromatic)

Individual category member substances are comprised of aliphatic hydrocarbon molecules with carbon numbers between C9 and C14; approximately 80% of the aliphatic constituents for a given substance fall within the C9-C14 carbon range and < 2% (although as shown in table, in most cases the levels of aromatics are well below 2%) of the total hydrocarbons present.

The substances in the C9-C14 Aliphatic [< 2% aromatic] Hydrocarbon Solvents Category contain >98% hydrocarbons. Several category members are described as UVCBs (Unknown or Variable Composition, Complex Reaction Products and Biological Materials) because they are composed of a defined, progressive carbon number range that includes various types of hydrocarbons: aliphatic molecules (linear, branched, and cyclic) and less than 2% aromatic molecules (generally one-ring alkylbenzenes), predominantly in the C9 to C14 range. The benzene and sulphur contents of substances in this category are low; benzene levels for example are typically < 3 ppm.

The substances and their identifiers are listed below:

HSPA Substance Name	CAS Number	EC Number
Hydrocarbons, C9-C11, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	919-857-5
Hydrocarbons, C9-C10, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	927-241-2

[3] Value taken from GaBi database, using Hexane as reference

Hydrocarbons, C9-C11, isoalkanes, cyclics, <2% aromatics	n.a.	920-134-1
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	918-481-9
Hydrocarbons, C10-C13, isoalkanes, cyclics, <2% aromatics	n.a.	918-317-6
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	926-141-6
Hydrocarbons, C13-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	917-488-4
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, cyclics, <2% aromatics	n.a.	920-107-4
Hydrocarbons, C11-C14, isoalkanes, cyclics, <2% aromatics	n.a.	927-285-2
Hydrocarbons, C10-C12, isoalkanes, <2% aromatics	n.a.	923-037-2
Hydrocarbons, C11-C12, isoalkanes, <2% aromatics	n.a.	918-167-1
Hydrocarbons, C11-C13, isoalkanes, <2% aromatics	n.a.	920-901-0
Hydrocarbons, C10-C13, n-alkanes, <2% aromatics	n.a.	929-018-5
Hydrocarbons, C11-C14, n-alkanes, <2% aromatics	n.a.	924-803-9
Hydrocarbons, C13-C14, n-alkanes, <2% aromatics	n.a.	939-519-0
Hydrocarbons, C10-C12, n-alkanes, <2% aromatics	n.a.	926-527-4
Hydrocarbons, C9-C11, cyclics, <2% aromatics	n.a.	925-894-8
Decane	124-18-5	204-686-4
Undecane	1120-21-4	214-300-6
Dodecane	112-40-3	203-967-9
Tridecane	629-50-5	211-093-4
Tetradecane	629-59-4	211-096-0
Isododecane (2,2,4,6,6-pentamethylheptane)	13475-82-6	236-757-0
Hydrocarbons, C4, 1,3-butadiene-free polymd, triisobutylene fraction, hydrogenated	93685-81-5	297-629-8
Hydrocarbons, C10-C14 (even numbered), n-alkanes, isoalkanes, <2% aromatics	n.a.	920-274-3
Hydrocarbons, C12-C16, isoalkanes, cyclics, < 2% aromatics	n.a.	927-676-8
Hydrocarbons, C8-C11, n-alkanes, isoalkanes, <2% aromatics	n.a.	940-733-1

Hydrocarbons, C9-C11, n-alkanes, isoalkanes, <2% aromatics	n.a.	941-718-2
Hydrocarbons, C9-C12, n-alkanes, isoalkanes, <2% aromatics	n.a.	940-725-8
Hydrocarbons, C10-C13, n-alkanes, isoalkanes, <2% aromatics	n.a.	940-726-3
Hydrocarbons, C11-C13 (odd number), n-alkanes, <2% aromatics	n.a.	942-924-5
Hydrocarbons, C11-C14, n-alkanes, isoalkanes, <2% aromatics	n.a.	701-280-3
Hydrocarbons, C11-C16, n-alkanes, isoalkanes, <2% aromatics	n.a.	942-085-5
Hydrocarbons, C12-C15, n-alkanes, isoalkanes, <2% aromatics	n.a.	940-727-9
Alkanes, C12-14 iso-	68551-19-9	271-369-5

As representative gross calorific value of 47,3 MJ/kg per solvent is approximated[4].

[4] Value taken from GaBi database, using Naphtha as reference

2.3 MANUFACTURING DESCRIPTION

The transformation of petroleum feedstocks into hydrocarbon solvent substances is a combination of various process steps that may include distillation of the feedstock, hydrodesulphurization, mild or heavy hydrogenation, and finally a distillation and a stripping of light components. Production process of the hydrocarbon solvents for each category is described below:

Category 3 solvents: White spirits

The various types and grades of white spirit are produced from straight-run kerosene, which are refinery streams obtained from the distillation of crude oil or condensate. These fractions are subjected to fractional distillation into appropriate boiling ranges and to hydrotreating process to obtain the desired type of white spirit. The composition of the white spirits may vary due to variation in the composition of the feedstocks and also because of the differences in refinery processing.

Category 6 solvents: Hexane solvents

Hexane solvents are produced from C6 rich naphtha, which is a refinery stream obtained from the distillation of crude oil. First, naphtha is desulfurized and fed to the benzene saturation process in contact with the catalyst. The reaction product is cooled, and the liquid fraction is distilled to separate the mixture of C6 isomers containing hexane.

Category 8 solvents: De-aromatized white spirits

De-aromatized white sprit has a very low level of aromatic compounds. The production process is similar to the white sprits including additionally de-aromatization (hydrotreating process unit, in which its aromatic compounds are hydrogenated) after desulphurization.

2.4 PRODUCER DESCRIPTION

Eco-profiles represent European industry averages within the scope of HSPA as the issuing trade federation. Hence, they are not attributed to any single producer, but rather to the European solvents industry as represented by HSPA'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		
		Cat. 3	Cat. 6	Cat. 8
ExxonMobil	ExxonMobil Petroleum and Chemical B.V.B.A Hermeslaan 2 1831 Machelen Belgium	X	X	X
Haltermann Carless	Haltermann Carless UK Ltd Refinery Rd Harwich CO12 4QG England	X		
Hellenic Petroleum	Hellenic Petroleum SA 8A Chimarras str., 15125 Maroussi Greece	X	X	
Shell	Shell Global Solutions GmbH Hohe-Schaar-Str. 36 21107 Hamburg Germany		X	X
TotalEnergies Fluids	TotalEnergies Fluids SAS 24 cours Michelet - La Défense 10 92069 Paris la Défense Cedex France		X	X

2.5 System Boundaries

PlasticsEurope Eco-profiles refer to the production of building blocks (in this case solvents) as a cradle-to-gate system (see Figure 1 for category 3, Figure 2 for category 6, and Figure 3 for category 8 solvents).

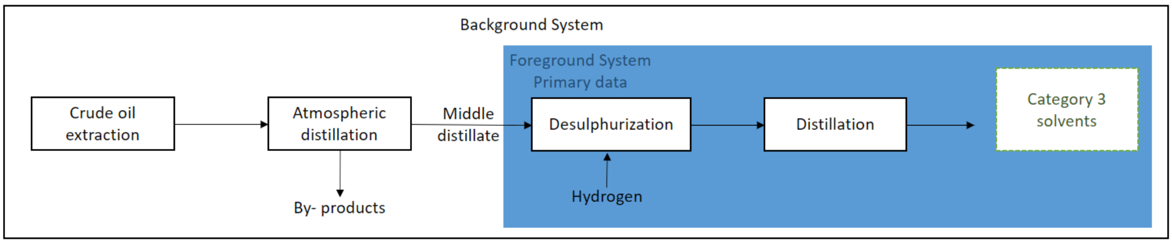

Figure 1: Cradle-to-gate system boundaries (Category 3)

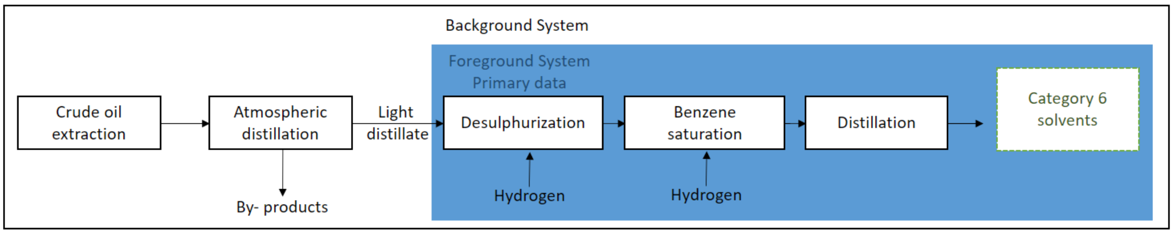

Figure 2: Cradle-to-gate system boundaries (Category 6)

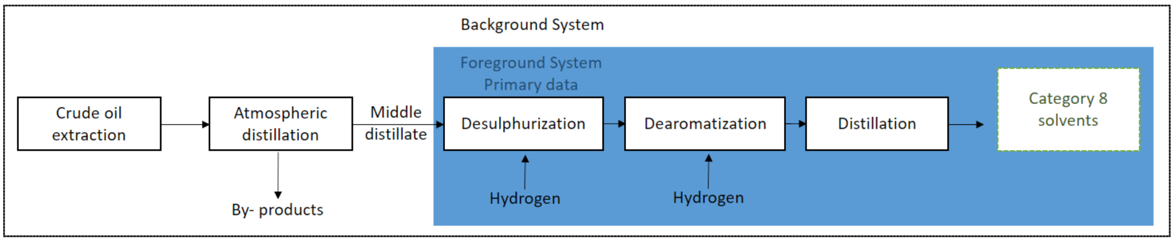

Figure 3 : Cradle-to-gate system boundaries (Category 8)

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 volumes produced in the European industry market in 2018 - according to qualified expert judgement by HSPA. So the generated datasets represent the average environmental burden of the participating companies.

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, 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. 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

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. All transports in the pre-chain contribute maximum 0.2% to the overall environmental burden.

In the foreground system all direct supply transports have been considered. No cut offs for auxiliaries and/or input flows with little consumption value has been conducted.

With regards to water use and consumption, some companies did not report any water inputs (for cooling and/or steam production purposes), as most vast majority of the water is considered to be relooped/recycled to the process again. As a consequence of this, the average relative water use/consumption reported by some companies has been assumed to be valid for each of the companies with regards to cooling water, while steam water losses were neglected, and steam condensate considered to be recycled.

2.10 DATA QUALITY REQUIREMENTS

Data Sources

Eco-profiles developed by HSPA 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 HSPA (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 applicable.[5]

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

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[5] Due to the project goal of developping 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).

conducted. The methodological framework is consistent throughout the whole model as the same methodological principles are used both in foreground and background system.

Reliability

Data reliability ranges from measured to estimated data. Data of foreground processes provided directly by producers were predominantly measured. 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 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).

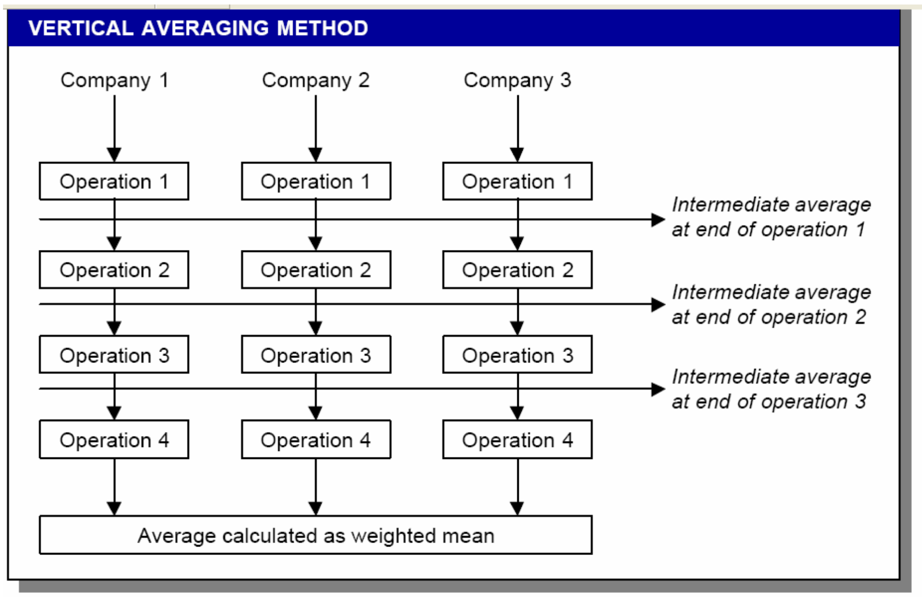

Figure 4: Vertical Averaging (source: Eco-profile of high-volume commodity phthalate esters, ECPI European Council for Plasticisers and Intermediates, 2001)

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.

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]).

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 (∆) 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 Cat. 3 solvents

Primary Energy Demand	**Value [MJ]**
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	47,30
Process energy (quantified as difference between primary energy demand and energy content of solvent)	7,42
Total primary energy demand	**54,72**

Table 2 Primary energy demand (system boundary level) per 1kg Cat. 6 solvents

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	48,10
Process energy (quantified as difference between primary energy demand and energy content of solvent)	10,48
Total primary energy demand	**58,58**

Table 3 Primary energy demand (system boundary level) per 1kg Cat. 8 solvents

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	47,30
Process energy (quantified as difference between primary energy demand and energy content of solvent)	9,78
Total primary energy demand	**57,08**

Water cradle to gate Use and Consumption

The cradle-to-gate[6] blue water **use** accounts for

- Cat. 3 solvents: 108,3 kg
- Cat. 6 solvents: 204,1 kg
- Cat. 8 solvents: 151,6 kg

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

- Cat. 3 solvents: 0,25 kg
- Cat. 6 solvents: 0,5 kg
- Cat. 8 solvents: 1,04 kg

[6] This includes water use in the total upstream supply chain

Water foreground (gate to gate) Use and Consumption[7]

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 Cat. 3 solvents

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	0,00	0,35	0,00	0,00	**0,35**
Untreated (from river/lake)	0,00	0,00	0,00	0,00	**0,00**
Untreated (from sea)	0,00	0,00	0,00	0,00	**0,00**
Relooped	0,00	0,00	0,00	0,00	**0,00**
Totals	**0,00**	**0,35**	**0,00**	**0,00**	**0,35**

Table 5 Water use and source per 1kg of Cat. 6 solvents

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	0,00	0,00	0,02	0,00	**0,02**
Untreated (from river/lake)	0,00	0,70	0,01	0,00	**0,72**
Untreated (from sea)	0,00	0,00	0,00	0,00	**0,00**
Relooped	0,00	0,21	0,00	0,00	**0,21**
Totals	**0,00**	**0,91**	**0,04**	**0,00**	**0,95**

Table 6 Water use and source per 1kg of Cat. 8 solvents

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0,00	0,71	0,00	0,00	**0,71**
Deionized / Softened	0,00	0,00	0,00	0,00	**0,00**
Untreated (from river/lake)	0,00	7,54	0,00	0,00	**7,54**
Untreated (from sea)	0,00	0,00	0,00	0,00	**0,00**
Relooped	0,00	1,77	0,00	0,00	**1,77**
Totals	**0,00**	**10,02**	**0,00**	**0,00**	**10,03**

[7] Due to data gaps with respect to water reporting these figures contain higher uncertainty.

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 Cat. 3 solvents

Treatment	**Water Output [kg]**
To WWTP	0,35
Untreated (to river/lake)	0,00
Untreated (to sea)	0,00
Relooped	0,00
Water leaving with products	0,00
Water Vapour	0,00
Formed in reaction (to WWTP)	0,00
Totals	**0,35**

Table 8 Treatment of Water Output per 1kg of Cat. 6 solvents

Treatment	**Water Output [kg]**
To WWTP	0,00
Untreated (to river/lake)	0,72
Untreated (to sea)	0,00
Relooped	0,23
Water leaving with products	0,00
Water Vapour	0,00
Formed in reaction (to WWTP)	0,00
Totals	**0,95**

Table 9 Treatment of Water Output per 1kg of Cat. 8 solvents

Treatment	**Water Output [kg]**
To WWTP	0,00
Untreated (to river/lake)	7,55
Untreated (to sea)	0,00
Relooped	1,77
Water leaving with products	0,00
Water Vapour	0,71
Formed in reaction (to WWTP)	0,00
Totals	**10,03**

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)

- Cat. 3 solvents = 0,00 kg
- Cat. 6 solvents = 0,00 kg
- Cat. 8 solvents = 0,71 kg

Dominance Analysis

The following tables show for each 1 kg of the products in scope of this study the contribution analysis to those LCI and LCIA indicators which were considered most relevant (see chapter 1.4)

As for all the product groups in scope of this study refinery products (from atmospheric distillation of crude oil) function as the main raw materials it might be worth to consider also the modelling and allocation principles applied for the creation of those main background datasets such as kerosene, naphtha, etc: https://sphera.com/wp-content/uploads/2020/04/The-GaBi-LCA-Refinery-Model.pdf

- Cat.3 solvents:

    - It can be observed that the consumed raw materials show an overwhelming contribution (with at least 91% in each of the impact categories except for the ozone depletion potential and eutrophication, freshwater category
    - The global warming potential shows a raw materials contribution of 95%, followed by the generation of the necessary thermal energy (4%). All other processes can be neglected regarding this impact category
    - Eutrophication shows an almost equal distribution of burden caused by the raw materials but also of the process waste treatment. This, relatively high share is mostly driven by cooling wastewater treatment.
    - The category ozone depletion is completely dominated by the electricity consumed. To be more precise, this is due to some dominating emissions related to the nuclear power consumption, which is still the main/ relevant share in some of the European grid mixes (Belgium) applicable to the considered producers mix of cat. 3 solvents. The same goes for utilities (20% contribution) which in this case is mostly compressed air (= another way of electricity consumption)
      As process waste treatment and potential credits of its thermal recovery consistently make use of the beforementioned grid mixes as well, there is also a relevant negative contribution to be seen which originate from these electricity credits
    - Other processes like infrastructure, transportation don´t show relevant contribution in any of the categories selected.

Table 10 Dominance analysis of impacts per 1kg Cat. 3 solvents

	Total Primary Energy	Resource use, energy carriers	Resource use, minerals and metals	Climate change, total	Acidification	Eutrophication, freshwater	Photochemical ozone formation	Ozone depletion
Production Process	0%	0%	0%	0%	0%	0%	8%	0%
Raw Materials	99%	99%	98%	95%	99%	51%	91%	1%
Thermal Energy	1%	1%	1%	4%	1%	0%	1%	0%
Electricity	0%	0%	0%	0%	0%	0%	0%	115%
Utilities	0%	0%	0%	0%	0%	3%	0%	20%
Process Waste Treatment	0%	0%	0%	0%	0%	45%	0%	-37%
Infrastructure	0%	0%	0%	0%	0%	0%	0%	1%
Transports	0%	0%	0%	0%	0%	0%	0%	1%
Total	100%	100%	100%	100%	100%	100%	100%	100%

- Cat.6 solvents:

    - It can be observed that the consumed raw materials show an overwhelming contribution (with at least 76% in each of the impact categories except for the ozone depletion potential
    - The global warming potential shows a raw materials contribution of 76%, followed by the generation of the necessary thermal energy (16%) and electricity (5%) and direct process emissions (2%). All other processes can be neglected regarding this impact category
    - The category ozone depletion is completely dominated by the electricity consumed. To be more precise, this is due to some dominating emissions related to the nuclear power consumption, which is still the main/ a relevant share in some of the European grid mixes (Belgium, France) applicable to the considered producers mix of cat. 6 solvents.
    - Other processes like infrastructure, utilities, process waste treatment and transportation don´t show relevant contribution in any of the categories selected.

Table 11 Dominance analysis of impacts per 1kg Cat. 6 solvents

	Total Primary Energy	**Resource use, energy carriers**	**Resource use, minerals and metals**	**Climate change, total**	**Acidification**	**Eutrophication, freshwater**	**Photochemical ozone formation**	**Ozone depletion**
Production Process	0%	0%	0%	2%	0%	0%	4%	0%
Raw Materials	94%	94%	93%	76%	96%	95%	90%	0%
Thermal Energy	4%	4%	5%	16%	3%	1%	5%	0%
Electricity	2%	2%	2%	5%	1%	3%	2%	100%
Utilities	0%	0%	0%	0%	0%	0%	0%	0%
Process Waste Treatment	0%	0%	0%	0%	0%	0%	0%	-1%
Infrastructure	0%	0%	1%	0%	0%	1%	0%	0%
Transports	0%	0%	0%	0%	0%	0%	0%	0%
Total	100%	100%	100%	100%	100%	100%	100%	100%

- Cat.8 solvents:

    - It can be observed that the consumed raw materials show an overwhelming contribution (with at least 91% in each of the impact categories except for the ozone depletion potential
    - The global warming potential shows a raw materials contribution of 91%, followed by the generation of the necessary thermal energy (7%) and electricity (1%) and direct process emissions (1%). All other processes can be neglected regarding this impact category
    - The category ozone depletion is almost completely (91%) dominated by the electricity consumed. To be more precise, this is due to some dominating emissions related to the nuclear power consumption, which is still the main/ a relevant share in some of the European grid mixes (Belgium, France) applicable to the considered producers mix of cat. 8 solvents.
    - Other processes like infrastructure, utilities, process waste treatment and transportation don´t show relevant contribution in any of the categories selected.

Table 12 Dominance analysis of impacts per 1kg Cat. 8 solvents

	Total Primary Energy	**Resource use, energy carriers**	**Resource use, minerals and metals**	**Climate change, total**	**Acidification**	**Eutrophication, freshwater**	**Photochemical ozone formation**	**Ozone depletion**
Production Process	0%	0%	0%	1%	0%	0%	1%	0%
Raw Materials	98%	98%	96%	91%	98%	94%	96%	8%
Thermal Energy	1%	1%	2%	7%	1%	1%	2%	0%
Electricity	0%	0%	2%	1%	0%	3%	0%	91%
Utilities	0%	0%	0%	0%	0%	1%	0%	1%
Process Waste Treatment	0%	0%	0%	0%	0%	0%	0%	0%
Infrastructure	0%	0%	0%	0%	0%	1%	0%	0%
Transports	0%	0%	0%	0%	0%	0%	0%	0%
Total	100%	100%	100%	100%	100%	100%	100%	100%

3 REVIEW

3.1 EXTERNAL INDEPENDENT REVIEW SUMMARY

DEKRA

Critical Review Statement

Eco-profile of three hydrocarbon solvent groups: Cat. 3 solvents, Cat. 6 solvents, Cat. 8 solvents

Commissioned by:	Hydrocarbon Solvent Producers Association (HSPA)
Version:	Eco-profile, October 2021
Prepared by:	Yannick Bernard, Sphera Solutions GmbH
Reviewed by:	Angela Schindler, DEKRA Assurance Services GmbH
References:	▪ 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)

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Geschäftsführer:
Matthias Witte

External independent review

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

- Cat. 3 solvents
- Cat. 6 solvents
- Cat. 8 solvents

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.

Each declared inventory cover a product family. From the life cycle assessment perspective, the processing of several substances of this type can be seen as comparable and thus can be described with the same life cycle inventory.

Due to the similar chemical structure the information on the calorific value, relevant for environmental performance in the End-of-life stage, but usually not for the production and application, is reduced to the information for a representative product of the product family.

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 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 mistakes 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 HSPA solvents

Indicator	Unit	Cat. 3 solvents	Cat. 6 solvents	Cat. 8 solvents
Climate change, total	kg CO_2 eq.	0,53	0,84	0,67
Climate Change, biogenic	kg CO_2 eq.	3,86E-04	3,07E-04	2,93E-04
Climate Change, fossil	kg CO_2 eq.	0,53	0,84	0,67
Climate Change, land use and land use change	kg CO_2 eq.	1,30E-04	1,54E-04	1,41E-04
Ozone depletion	kg CFC-11 eq.	9,79E-13	1,46E-11	1,04E-11
Acidification	Mole of H+ eq	2,80E-03	3,54E-03	2,94E-03
Photochemical ozone formation	kg NMVOC eq	2,09E-03	2,47E-03	2,07E-03
Eutrophication, freshwater	kg P eq	1,03E-06	9,54E-07	6,15E-07
Eutrophication, marine	kg N eq.	4,08E-04	5,10E-04	4,43E-04
Eutrophication, terrestrial	Mole of N eq.	4,48E-03	5,65E-03	4,89E-03
Respiratory Inorganics	Disease incidences	1,73E-08	2,18E-08	1,83E-08
Ionising radiation, human health	kBq U235 eq.	0,01	0,02	0,01
Human toxicity, cancer - total	CTUh	4,01E-10	4,55E-10	4,08E-10
Human toxicity, cancer inorganics	CTUh	9,14E-22	2,06E-21	1,18E-21
Human toxicity, cancer metals	CTUh	3,46E-10	3,56E-10	3,45E-10
Human toxicity, cancer organics	CTUh	5,48E-11	9,83E-11	6,28E-11
Human toxicity, non-cancer - total	CTUh	1,44E-08	1,52E-08	1,47E-08
Human toxicity, non-cancer inorganics	CTUh	5,93E-09	6,14E-09	5,94E-09
Human toxicity, non-cancer metals	CTUh	8,37E-09	8,99E-09	8,69E-09
Human toxicity, non-cancer organics	CTUh	2,63E-10	2,89E-10	2,68E-10
Ecotoxicity, freshwater - total	CTUe	3,52E+01	3,51E+01	3,47E+01
Ecotoxicity, freshwater inorganics	CTUe	3,44E+01	3,42E+01	3,39E+01
Ecotoxicity, freshwater metals	CTUe	5,66E-01	6,78E-01	6,15E-01

Ecotoxicity, freshwater organics	CTUe	2,32E-01	2,32E-01	2,28E-01
Land Use	Pt	1,32E-01	7,22E-01	3,98E-01
Resource use, energy carriers	MJ	50,86	54,26	52,94
Resource use, minerals and metals	kg Sb eq.	1,03E-07	1,14E-07	1,10E-07
Water scarcity	m^3 world equiv.	2,39E-03	1,52E-02	1,02E-02

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