

Eco-profile
of n-Butyl Acetate
December 2024

1 SUMMARY

This Eco-profile report has been prepared according to the **Eco-profiles program and methodology – PlasticsEurope – V3.1 (2022)** 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 1 kg of **n-Butyl Acetate** analysed from cradle to gate (from crude oil extraction to liquid solvent 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 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
Representativeness	Up to 100% of European production
Reference year	2022
Year of data collection and calculation	2023/2024
Expected temporal validity	Revision should be considered in 2029
Cut-offs	No significant cut-offs
Data Quality	Very good
Allocation method	Not applicable

1.2 DESCRIPTION OF THE PRODUCT AND THE PRODUCTION PROCESS

This Eco-profile is for the oxygenated solvent n-Butyl Acetate. Oxygenated solvents are organic solvents, their molecules contain oxygen. They 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 show good solvency performance and are wholly or partly miscible with water.

n-Butyl Acetate, also known as butyl ethanoate, is a colourless and flammable solvent with a fruity odour. It has excellent solvency characteristics for polymers, resins, oils and cellulose nitrate and is miscible with common organic solvents.

The reference flow, to which all data given in this Eco-profile refer, is 1 kg of n-Butyl Acetate.

Production Process

The process to produce n-Butyl Acetate is based on the esterification of Butanol with Acetic Acid. The use of Butanol and Acetic Acid results in the formation of water which is continuously removed in order to shift the equilibrium and enhance the ester formation.

Use Phase and End-of-Life Management

n-Butyl Acetate is used as a solvent in organic chemistry. As a solvent, it is used for example in paints, varnishes, fats, oils and polymers. Other uses include coating fabric in the textiles industry, as a cleaning or polishing agent and in consumer products such as make-up and nail products, and fragrance solvents. The main user end market of this product is paints, varnishes and coatings.

With regards to the End-of-Life (EoL) treatment of this solvent, of course, no general statements can be made as it is clearly depending on its 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 solvent/ 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 three European producers: 3 plants from 2 different countries.

For the solvent in scope of this study, primary production data covers about 100% of the European n-Butyl Acetate production capacity, according to qualified expert judgement by OSPA.

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 EF 3.1 compliant

datastock [EF DATABASE 2022] , whenever applicable. Sphera's managed LCA Content (MLC) databases (formerly, GaBi database) [SPHERA 2023] were used to close the gap for those relevant background dataset which are not available from the EF compliant database. Most of the background data used is publicly available and public documentation exists. For Butanol, primary production data for each of the participating companies was used (the data was previously collected for the n-Butanol Eco-profile report (EF 3.0 compliant dataset)) [ESIG 2021].

No allocation had to be applied in the foreground systems of the products in scope.

1.4 ENVIRONMENTAL PERFORMANCE

The tables below show the environmental performance indicators associated with the production of 1 kg of n-Butyl Acetate solvent. Please refer to chapter 4 for a complete overview of all EF 3.1 indicator results of the solvent in scope.

1.4.1 Input Parameters

Indicator	Unit	Value	Impact method ref.
Non-renewable energy resources ¹⁾			
• Fuel energy	MJ	57.33	-
• Feedstock energy	MJ	30.5 ¹⁾	Gross calorific value
Renewable energy resources (biomass) ¹⁾			
• Fuel energy	MJ	3.55	-
• Feedstock energy	MJ	0.00	Gross calorific value
Resource use			
• Minerals and Metals	kg Sb eq.	4.09E-06	EF 3.1
• Energy Carriers	MJ	81.08	EF 3.1
Renewable materials (biomass)	kg	0	-
Water use	m ³ world eq.	0.47	EF 3.1
¹⁾ Calculated as upper heating value (UHV)			

1.4.2 Output Parameters

Indicator	Unit	Value	Impact method ref.
Climate change, total	kg CO ₂ eq.	3.04	EF 3.1
Ozone depletion	kg CFC-11 eq.	5.55E-10	EF 3.1
Acidification	Mole of H ⁺ eq.	6.63E-03	EF 3.1
Photochemical ozone formation	kg NMVOC eq.	6.17E-03	EF 3.1
Eutrophication, freshwater	kg P eq.	8.15E-05	EF 3.1
Respiratory Inorganics	Disease incidences	7.21E-08	EF 3.1
Waste			
• Non-hazardous	kg	0.50	-
• Hazardous	kg	3.46E-04	-

¹⁾ Estimated from literature [CAMEO CHEMICALS 1999].

1.5 PROGRAMME OWNER

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2 ECO-PROFILE REPORT

2.1 FUNCTIONAL UNIT AND DECLARED UNIT

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

2.2 PRODUCT DESCRIPTION

- IUPAC name: Butyl Acetate
- CAS numbers covered in this study: 123-86-4
- chemical formula: $C_6H_{12}O_2$
- gross calorific value: 30.5 MJ/kg

2.3 MANUFACTURING DESCRIPTION

n-Butyl Acetate is produced via esterification of Butanol and Acetic Acid, in the presence of a catalyst. The synthesis reaction is a reversible reaction whereby Butanol is heated with Acetic Acid in the presence of the catalyst to produce n-Butyl Acetate and water. The produced water from the reaction is continuously removed to shift the equilibrium and enhance the ester formation.

Reaction scheme:



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
BASF	BASF SE Carl-Bosch-Strasse 38 67056 Ludwigshafen Germany
INEOS Oxide	INEOS Oxide Avenue des Uttins 3 Rolle 1180 Switzerland
OQ	OQ Chemicals GmbH Rheinpromenade 4a 40789 Monheim am Rhein Germany

2.5 SYSTEM BOUNDARIES

The Eco-profile refers to the production of n-Butyl Acetate solvent as a cradle-to-gate system (see Figure 1). In a preceding Eco-profile project [ESIG 2021], the participating companies of this study have also reported primary data for the production of n-Butanol. The resulting life cycle inventories are now used as upstream background dataset for this study. The diagram shows the common foreground and background system.

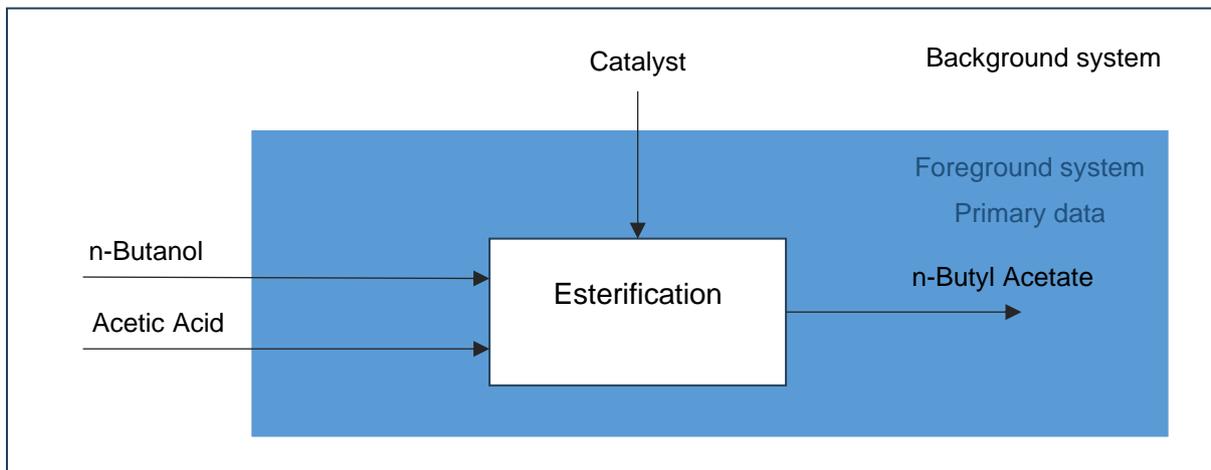


Figure 1: Cradle-to-gate system boundaries (n-Butyl Acetate)

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 the defined production region of the participating producers. The considered participants cover about 100% of European production in 2022 (according to qualified expert judgement by OSPA) in the reference year mentioned above.

Primary data were used for all foreground processes (under operational control) and the life cycle inventory (background data) for n-Butanol, which is one of the main precursors in the production of n-Butyl acetate. Primary data was 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 2022.

Background data have reference year from 2022 (Sphera data), and 2012-2017 regarding the EF 3.1 datasets. For n-Butanol, the background data have the reference year from 2019 (Sphera data), and 2012/2015 regarding the EF 3.0 datasets [ESIG 2021].

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 2022 with a recommended temporal validity until 2029.

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

In the foreground processes all reported flows were considered

According to the Managed LCA Content MLC 2023 (formerly, GaBi database) [SPHERA 2023], and EF compliant datasets [EF DATABASE 2022] 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 MLC 2023 LCI database (formerly, GaBi database) [SPHERA 2023] of the software system Sphera LCA for Experts “LCA FE” (formerly, GaBi software) and the officially available EF compliant datasets [EF DATABASE 2022], 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 100% of the European industry market (2022) regarding the solvent 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 Managed LCA Content 2023 (formerly GaBi databases) [SPHERA 2023] and the officially available EF compliant datasets [EF DATABASE 2022] 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

² Due to the project goal of developing EF 3.1 compliant datasets, the background datasets need to be taken from the current version of the EF Reference Package (v3) (with the reference year 2012-2015 for energy datasets).

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 MLC (formerly, GaBi) data or EF compliant 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 LCA For Experts (formerly, GaBi 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 MLC database (formerly GaBi databases) [SPHERA 2023] 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 LCA For Experts (formerly GaBi). The associated database integrates ISO 14040/44 requirements. LCA modelling has been carried out following the rules of EF 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 2).

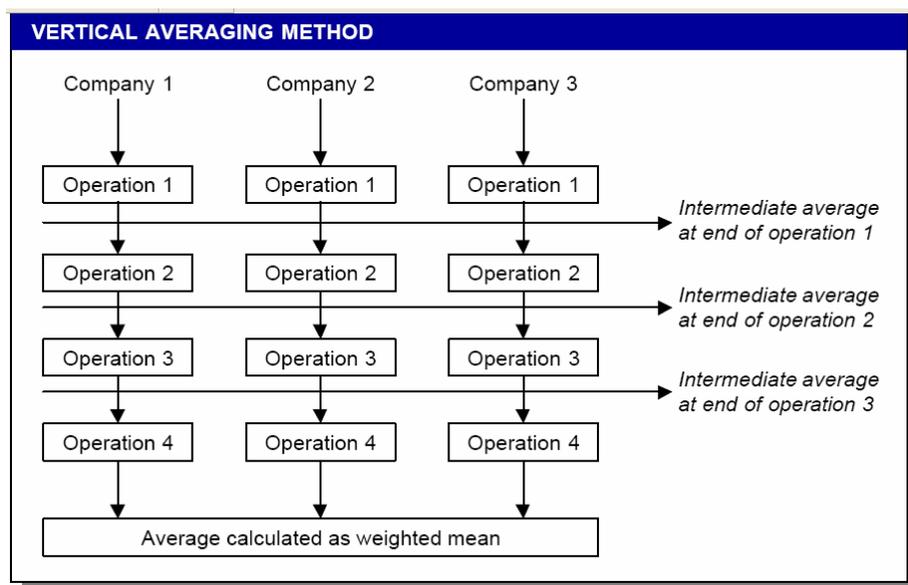


Figure 2: Vertical Averaging Method

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.

Foreground system:

No allocation had to be applied in the foreground systems of the products in scope.

Background system:

Regarding the used background datasets from Sphera's MLC databases, in the refinery operations, co-production was addressed by applying allocation based on mass and net calorific value [SPHERA 2023] 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 3.1 compliant dataset per average solvent in ILCD/EF 3.1 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.
- LCA for experts format (.GabiDB)
- 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 solvent** 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-Butyl Acetate

Primary Energy Demand	Value [MJ]
Energy content in solvent (energy recovery potential, quantified as gross calorific value of solvent)	30.5
Process energy (quantified as difference between primary energy demand and energy content of solvent)	60.88
Total primary energy demand	91.38

Water cradle to gate Use and Consumption

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

- n-Butyl Acetate: 2981.4 kg

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

- n-Butyl Acetate: 25.3 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 2 Water use and source per 1kg of n-Butyl Acetate

Source	Process water [kg]	Cooling water [kg]	Steam Water [kg]	Water in Raw Materials [kg]	Total [kg]
From Tap	0.00	1.91	0.00	0.00	1.91
Deionized / Softened	0.01	0.00	1.45	0.00	1.46
Untreated (from river/lake)	0.00	7.95	0.00	0.00	7.95
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	0.01	9.85	1.45	0.00	11.32

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

³ This includes water use in the total upstream supply chain

Table 3 Treatment of Water Output per 1kg of n-Butyl Acetate

Treatment	Water Output [kg]
To WWTP	0.01
Untreated (to river/lake)	0.00
Untreated (to sea)	0.00
Re looped	11.30
Water leaving with products	0.00
Water Vapour	0.00
Formed in reaction (to WWTP)	0.16
Totals	11.46

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-Butyl Acetate = - 0.156 kg

The water consumption value for n-Butyl Acetate is negative as a result of water generation during the synthesis of the solvent via esterification.

3 REVIEW

3.1 EXTERNAL INDEPENDENT REVIEW SUMMARY



Critical Review Statement *Eco-profile of n-Butyl Acetate*

DEKRA Alles im grünen Bereich

Commissioned by:	Oxygenated Solvent Producers Association (OSPA) Hydrocarbon Solvent Producers Association (HSPA)
Version:	Eco-profile, November 2024
Prepared by:	Sphera Solutions GmbH, Abdessamad El Bahraoui
Reviewed by:	Angela Schindler Accredited partner of DEKRA Assurance Services GmbH
References:	<ul style="list-style-type: none">▪ ISO 14071 (2016): Environmental management – Life cycle assessment – Critical review processes and reviewer competencies: Additional requirements and guidelines to ISO 14044:2006▪ 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 v3.1 (2022)▪ Guide for EF compliant data sets v2.0 (2020)

EXTERNAL INDEPENDENT REVIEW

This Eco-profile covers the declaration of the environmental performance of the oxygenated solvent n-Butyl Acetate.

The Eco-profile document was submitted in August 2024; the review process was finalized in November/December 2024.

In principle, this document is a supplement to Eco-profile of OSPA, published in November 2021.

The compliance of the document was reviewed according to the current requirements of the Eco-profiles program and methodology, version 3.1 (2022) of PlasticsEurope. Besides, the substantial intention of this Eco-profile is the generation of a life cycle inventory for the above-mentioned substance, 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, with this review statement it is confirmed, that 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 comprised the check of the Eco-profile document, a discussion of data input, software model and detailed assessment in a webmeeting with the LCA practitioner and the check of the obligatory files for generating the life cycle inventories to be provided for the PEF background database.

All comments of the reviewer could be solved in the webmeeting and by implementing respective adaptations to the Eco-profile report.

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.

The data quality is assessed according to the DQR requirements. The details have been shown to the reviewer; the final result of the DQR procedure is published in the documentation of the life cycle inventory.

The participants of the study confirmed that the applied raw materials are solely based on fossil resources (acetic acid). Thus, additional information on biogenic C-content is not necessary.

The data collection partly lacks the information on direct emissions of the process; due to the fact, that the declared values of other participants does not lead to significant contributions of the environmental indicators, this data gap is assessed as subordinated.

The mass balance has been checked and evaluated as sufficiently complete. The relatively high water use of the product can be explained by the supply chain of the input materials.

Due to the intention to generate a PEF-conform LCI, the software model integrates only official background data of the EF database of the European Commission, as far as they are available, supplemented with datasets of the current MLC database. As the EF 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 regarding the dynamically changing electricity grid mixes; in the current study the contribution of electricity can be seen as a minor contributing factor.

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

Overall, the project is carried out very thoroughly. The structure and description of the Eco-profile is clear and transparent, thus displaying a reliable source of information.

Salem, 03.12.2024



Angela Schindler

Approved partner of DEKRA Assurance Services GmbH, Stuttgart, Germany

3.2 REVIEWER CONTACT DETAILS

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4 EF 3.1 INDICATOR RESULTS

The following table shows the full list of EF 3.1 indicator results for n-Butyl Acetate :

Table 5: EF 3.1 indicator results for n-Butyl Acetate solvent

Indicator	Unit	Value
Climate change, total	kg CO ₂ eq.	3.04E+00
Climate Change, biogenic	kg CO ₂ eq.	6.01E-03
Climate Change, fossil	kg CO ₂ eq.	3.04E+00
Climate Change, land use and land use change	kg CO ₂ eq.	1.23E-03
Ozone depletion	kg CFC-11 eq.	5.55E-10
Acidification	Mole of H ⁺ eq.	6.63E-03
Photochemical ozone formation	kg NMVOC eq.	6.17E-03
Eutrophication, freshwater	kg P eq.	8.15E-05
Eutrophication, marine	kg N eq.	1.53E-03
Eutrophication, terrestrial	Mole of N eq.	1.66E-02
Respiratory Inorganics	Disease incidences	7.21E-08
Ionising radiation, human health	kBq U235 eq.	2.42E-01
Human toxicity, cancer – total	CTUh	9.36E-10
Human toxicity, cancer inorganics	CTUh	6.79E-10
Human toxicity, cancer organics	CTUh	2.57E-10
Human toxicity, non-cancer – total	CTUh	2.93E-08
Human toxicity, non-cancer inorganics	CTUh	2.56E-08
Human toxicity, non-cancer organics	CTUh	3.65E-09
Ecotoxicity, freshwater – total	CTUe	3.45E+01
Ecotoxicity, freshwater inorganics	CTUe	3.39E+01
Ecotoxicity, freshwater organics	CTUe	5.34E-01
Land Use	Pt	3.92E+00
Resource use, energy carriers	MJ	8.11E+01
Resource use, minerals and metals	kg Sb eq.	4.09E-06
Water use	m ³ world eq.	4.70E-01

5 REFERENCES

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