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Safe and Sustainable by Design chemicals and materials

Application of the SSbD framework to case studies

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Contents

Abstract

This report presents the first application of the European Commission (EC) Safe and Sustainable by Design (SSbD) framework in a case study, on plasticisers in food contact material. Both the SSbD framework and the case study were developed by the EC's Joint Research Centre. The case study was undertaken to elucidate possibilities for further refinements of the SSbD framework, and to enable its wider application to support innovation for safety and sustainability. Furthermore, two more case studies were developed in parallel by the industry, one that assessed flame retardants (halogen-free) in information and communications technology products, and one that focused on surfactants in textiles. Lessons learned and challenges were extracted from the case studies. A main challenge relates to lack of publicly available data in all steps of the assessment, as well as databases to act as repositories for this data. For example, for the safety aspects in Step 1 data used for classification purposes is Business Confidential Information, in Step 2 the manufacturing and processing are very company specific processes, or in Step 3 product/application specific and very often confidential information as well. For the life cycle assessment, detailed data regarding the production processes is required and it was not possible to obtain it from companies neither in general life cycle databases. Furthermore, data quality and uncertainty is important, and need to be addressed. It was noted that the integration of different disciplines (e.g. risk assessment, lifecycle assessment) enables a very comprehensive assessment, however such expertise is not easily found pointing out for the need of training on SSbD to develop the necessary skills. Nevertheless, the assessment is complex and requires the assessor(s) to have expertise in various fields, which can be particularly challenging for small and medium enterprises. A need was identified for additional case studies to support further developments towards operationalization of the EC SSbD framework, including its alignment with companies design and innovation processes. Additionally, to successfully implement the SSbD framework it is key to develop a system enabling the communication along the supply chain of the information necessary to conduct the assessment.

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Disclaimer

This report aims at illustrating the application of the SSbD framework with a case study developed by the JRC with the support of several companies which shared information regarding the appropriate application (the gasket) and the production processes of the plasticiser.

Authors' contribution

Carla Caldeira: conceptualization, methodology, formal analysis writing-original. **Irantzu Garmendia Aguirre**: conceptualization, methodology, formal analysis, writing-original. **Davide Tosches:** methodology, formal analysis, writing-original**. Lucia Mancini:** methodology, formal analysis writing-original **Elisabetta Abbate**: writing – review and editing. **Lucian Farcal:** writing review and editing. **Dorelia Lipsa**: formal analysis. **Kirsten Rasmussen**: review and editing. **Hubert Rauscher**: review and editing. **Juan Riego Sintes**: review and editing. **Serenella Sala**: conceptualization, writing - review and editing, supervision, scientific project responsible at the JRC.

Executive summary

Context

The European Union's Chemicals Strategy for Sustainability (CSS) aims to catalyse the shift towards chemicals, materials and products that are safe and sustainable by design (SSbD) throughout their life cycles, i.e. from resources extraction to end-of-life management. Developing SSbD criteria for chemicals and materials is one of the key actions foreseen in the CSS, contributing to reducing negative impacts on human health and the environment associated with chemicals, materials, products and services produced, used or marketed in the EU. To support the CSS implementation concerning SSbD, the European Commission's Joint Research Centre (EC-JRC) developed a **framework for the definition of SSbD criteria** for **chemicals and materials**. The framework puts together safety, environmental and socio-economic dimensions of sustainability.

The JRC framework was the basis for the **EC Recommendation establishing a European assessment framework for safe and sustainable by design chemicals and materials** (EC SSbD recommendation) that is addressed to Member States, industry, academia and research and technology organisations. The framework should make it possible to comprehensively assess the safety and sustainability of chemicals and materials throughout their life cycle and support the design, development, production, and use of chemicals and materials that provide a desirable function while being safe and sustainable. This Recommendation sets a testing period for the framework to receive inputs from stakeholders regarding applicability and challenges encountered.

This report presents the **first application of the EC SSbD recommendation to case studies** on selected chemicals. This work was presented at the 3rd SSbD stakeholder workshop and the relevant recordings are available here: day 1[1] and day 2[2]. The case studies allowed to **increase the knowledge on the applicability of the framework** and to **support further refinement** thereof, as well as to advance the definition of criteria for SSbD.

Application of the proposed framework for SSbD chemicals and materials to case studies

The SSbD framework consists of two phases: 1) **Design (or re-design) phase**, where guiding design principles are proposed to support the development of safe and sustainable chemicals and materials, and 2) **Safety and sustainability assessment phase,** where the safety and sustainability of the chemical(s) or material(s) in question are assessed. The case studies were performed on selected **existing chemicals** and focussed on phase 2, namely on their safety and sustainability assessment.

Case study 1 Plasticiser (non-phthalate) in food contact material

A case study was developed addressing plasticisers already on the market and simulated a situation in which a chemical of concern was identified and would need to be substituted. The SSbD framework was applied to assess the safety and sustainability performance of the chemical to be substituted and the alternatives, performing a comparative assessment. The **chemical of concern** identified was di(2-ethyl hexyl) phthalate (DEHP) and the **five alternatives** are acetyl tributyl citrate (ATBC), di(2-ethyl hexyl) adipate (DEHA), di(2-ethyl hexyl) terephthalate (DEHT), di-isononyl cyclohexanoate (DINCH), and epoxidised soybean oil (ESBO). To apply the framework, a **specific use** needs to be defined which implies the selection of a product in which the plasticiser is used. After consultation with several stakeholders, and based on their feedback on current market application and data availability, the selected product was a sealing **gasket** made of a plastic liner placed below the metal cap in glass jars. The SSbD concept adopts a life cycle perspective, therefore the entire **life cycle of the plasticiser** was considered. Specifically, the safety and sustainability assessment of the sealing gasket consists of four steps:

Step 1: Hazard assessment of the chemical/material. In this step, a hazard assessment was performed using existing available data. The assessment illustrates the process of gathering available data/information, the identification of data gaps and how these in some cases can be justified. Finally, it also provides examples on considerations when generating data using alternative data sources and NAMs.

Step 2: Human health and safety aspects in the chemical/material production and processing phase. In this step, safety aspects related to the exposure to the plasticisers during the production and processing were

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[1] https://www.youtube.com/watch?v=0cGydn2wyE0
[2] https://www.youtube.com/watch?v=SKTrtKrAr6Y

assessed. Due to the high uncertainty on what happens at the end-of-life of the gasket and how to assess it, this stage has not been assessed. Although using conservative assumptions, the assessment illustrates that the exposure is a key aspect in the safety assessment and that in certain processes the high risk potential due to hazard properties can be reduced to a safety level, using - among other - risk management measures.

Step 3: Human health and environmental aspects in the "final application" phase. In this step, the safety during the gasket application was assessed. The assessment illustrates the difficulties due to the specificity of the case study. Furthermore, it also presents the considerations and different approaches that can be followed during the assessment to be able to draw certain conclusions.

Step 4: Environmental sustainability assessment. In this step, a life cycle assessment was performed. None of the alternatives performed sufficiently better than the reference used for all the impact categories, with the exception of ESBO for the impact category 'resources use fossil' due its bio-based nature. Nonetheless, the LCA results could support the chemical producer to improve the environmental performance as it allows identifying what are the most impactful impact category, life cycle stage, and process to be improved. An example on how to use this information in the re-design of a chemical/material production process is provided.

Furthermore, **exploratory approaches to social and economic sustainability assessment** along the chemical life cycle are proposed in **Step 5** to address.

An **illustrative scoring system** was developed with scores from 0 to 3, considering "SSbD" a minimum score of "2", to support decision making and facilitate the communication of results. An aggregation method that does not allow compensation was used with underpinning rules that can be adjusted to reflect the degree of ambition on the application of the framework.

Case studies developed by industries

Two case studies were developed by industries. **Case study 2** on flame retardants (halogen-free) in information and communication technology products, was developed by Clariant and BASF, **comparing halogenated flame retardants with non-halogenated ones**. **Case study 3** on surfactants in textiles was developed by Novozymes**, assessing an enzyme (pectate lyase)** that is used for scouring of cotton yarns and fabrics in the textile industry reducing energy and chemical consumption in a scouring process._The participation of these companies was **very welcomed and appreciated** as it allowed to have a first feedback from companies implementing the framework. Main **challenges** identified include the **high resources needs to perform the assessment**, **lack of data**, and the need for training and skills development to enable SSbD assessment. Despite these challenges, companies see a benefit in implementing the SSbD concept and are willing to explore its integration in their research and development strategies.

Lessons learnt

The development of these case studies shed light on relevant aspects for the application of the SSbD framework. There is, however, a **need for additional case studies** that can support further developments towards operationalization of the EC SSbD framework. It is relevant to further explore the **integration of the SSbD assessment with the design and innovation processes.** Stakeholders suggested to explore the development of a **tiered approach** that should not compromise the comprehensiveness and ambitions of the framework and the CSS. In order to better support the SSbD assessment throughout the development of chemicals/materials, there is the necessity to **explore the possibility of integrating the Risk Assessment and Life Cycle Assessment even further.** The combination of different disciplines enables a very comprehensive assessment, and requires a team effort by assessors with **expertise in various fields**.

A key and overarching challenge for all the steps is the availability of data; either the data does not exist (the case of new chemicals and materials) or it does but is not publicly available (chemicals and materials on the market). Data on new chemicals can be developed by means of robust predictive models and related platforms for data sharing. For chemicals on the market, data availability depends significantly on the willingness of stakeholders to share their data and the implementation of communication mechanisms throughout the value chain ensuring confidentiality. **Databases** with the relevant data for designing and assessing chemicals according to the proposed SSbD framework could be **developed with the collaboration of the stakeholders**, taking into account already existing databases. **Data quality and uncertainty** is a concern and data quality assessment should be included and taken into account in the assessment and subsequent decision making. Aside these aspects, for a successful implementation of the SSbD framework it is key to develop a **system enabling the communication along the supply chain** which will guaranteed the access to necessary information for conducting the assessment.

1 Introduction

1.1 Policy context

With the **European Green Deal** (EC, 2019) the European Commission aims to transform the European Union's (EU) economy to support a more sustainable future and to implement the United Nation's 2030 Agenda for Sustainable Development and the Sustainable Development Goals (SDGs). These include public health and environmental safety as integral elements of sustainable development. The European Green Deal, European Union's new growth strategy, has set the EU on a course to become a sustainable, climate neutral and circular economy by 2050. It has also set a goal to better protect human health and the environment as part of an ambitious approach to tackle pollution from all sources and move towards a toxic-free environment[3].

One of the key objectives of the European Green Deal is the **Zero Pollution Ambition**. The zero pollution vision for 2050 is for air, water and soil pollution to be reduced to levels no longer considered harmful to health and natural ecosystems that respect the boundaries with which our planet can cope, thereby creating a toxic-free environment. The headline actions on zero pollution include:

- **Chemicals strategy for sustainability** (CSS) (EC, 2020b) - which, among other, has an objective to better protect citizens and the environment against hazardous chemicals.
- **Zero pollution action plan for water, air and soil** (EC, 2021b) - to better prevent, remedy, monitor and report on pollution.
- Revising measures to address **pollution from large industrial installations** - to ensure they are consistent with climate, energy and circular economy policies.

The **CSS** (EC, 2020b) aims to catalyse the shift towards chemicals, materials and products that are "safe and sustainable by design" (SSbD) throughout their life cycles, i.e. from resources extraction to end-of-life management. Developing SSbD criteria for chemicals and materials is one of the key actions foreseen in the CSS, contributing to reducing possible negative impacts on human health and the environment associated with chemicals, materials, products and services produced, used or marketed in the EU.

1.2 The SSbD framework

To support the CSS implementation for what concerns SSbD, the European Commission's Joint Research Centre (EC-JRC) performed a **review** of existing frameworks (Caldeira et al., 2022a) compiling safety and sustainability dimensions, aspects, methods, indicators and tools, and developed a **framework for the definition of SSbD criteria** and evaluation procedure for **chemicals and materials** (Caldeira et al., 2022b). The framework puts together safety, environmental and socio-economic dimensions of sustainability. It should contribute to achieving the related Green Deal ambitions, while promoting innovation and a circular economy. Also, it should facilitate the design and development of safe and sustainable chemicals and materials from the early stages of innovation and along their entire life cycle. The SSbD framework proposes a hierarchical approach in which the safety aspects are considered first, followed by environmental and socio-economic aspects. The SSbD framework aims at:

- Promoting the application of the SSbD approach to chemicals and materials and steering innovation towards the green industrial transition;
- Enabling criteria development for the design and evaluation of 'safe' and 'sustainable' chemicals/materials;
- Driving innovation towards the substitution, or minimisation of the use, of substances of concern from production and use, in line with and beyond existing and upcoming regulatory obligations;
- Minimising or, eliminating the possible adverse impact on human health, climate and the environment (air, water, soil, biota) along the entire chemical's and material's life cycle;
- Enabling comparative assessment of chemicals and materials based on safety and sustainability performance for a given function or application context.

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[3] The Chemicals Strategy for Sustainability sets out the steps to take to achieve a toxic-free environment, and ensure that chemicals are produced and used in a way that maximises their contribution to society while avoiding harm to the planet and to current and future generations. The Strategy foresees that the most harmful chemicals are avoided for non-essential societal use, and that all industrial chemicals are used more safely and sustainably." (https://ec.europa.eu/commission/presscorner/detail/en/qanda_20_1840)

This work was the basis of the **EC Recommendation establishing a European assessment framework for safe and sustainable by design chemicals and materials** (EC, 2022a) that is addressed to Member States, industry, academia and research and technology organisations. The main purpose of the Recommendation is to test the framework and get feedback to be able to improve its relevance, reliability and operability. Moreover, the framework is seen as a central pillar of the **Strategic Research and Innovation Plan (SRIP)** for safe and sustainable chemicals and materials (EC, 2022b), which highlights current research and innovation (R&I) areas crucial for accelerating the transition to chemicals and materials that are safe and sustainable.

1.3 Objectives of the study

The main objective of this work was to evaluate the feasibility and applicability of the framework in assessments of selected chemicals via the development of case studies, namely on non-phthalate plasticisers (developed by the JRC) and halogen-free flame retardants and surfactants (both developed by industry). This work allowed to **assess the methodology proposed in the framework and its feasibility**, e.g. valuate if there are any overlapping aspects between the different assessment steps, mapping underpinning data used in each step, pinpoint limitations in the framework application, identify and compare relevant tools that can be used and establish data needs or gaps. Finally, such case studies covering several types of chemicals or materials should **provide additional knowledge** and support further refinement of the framework and advance on SSbD criteria definition.

This report presents the outcomes of the first set of SSbD case studies developed by the JRC in collaboration with experts and stakeholders, as a follow-up of the two previous JRC Technical Reports mentioned above (Caldeira et al., 2022b; Caldeira et al., 2022a) The report is also a result of the information exchange and interactions with stakeholders and experts after the publication of the framework.

1.4 Application of the proposed framework for SSbD chemicals and materials to case studies

The SSbD framework includes two phases **1) Design (or re-design) phase** at which guiding design principles are proposed to support the development of safe and sustainable of chemicals and materials, and **2) Safety and sustainability assessment phase,** in which the safety and sustainability of the chemical(s) or material(s) in question are assessed. The case studies were performed on existing chemicals being the main focus on the safety and sustainability assessment of the selected chemicals. The guiding principles of phase 1 were used to propose actions that could improve the performance of the chemicals on a design perspective.

The framework proposed a stepwise approach for the safety and sustainability assessment, composed of four steps:

- Step 1: Hazard assessment of the chemical/material, in which the intrinsic properties of the chemical or material are assessed to understand their hazard potential;
- Step 2: Human health and safety aspects in the chemical/material production and processing phase, where health and safety aspects related to the chemical/material production and processing are assessed;
- Step 3: Human health and environmental aspects in the “final application” phase, concerning the application/use-specific exposure to the chemical/material and the associated risks, both for human health and the environment;
- Step 4: Environmental sustainability assessment, assessing impacts along the entire chemical/material life cycle due to emissions into air, water and soil and due to resource use. This step is performed by means of Life Cycle Assessment (LCA).

Furthermore, Caldeira et al. (2022b) propose in Step 5 approaches to address social and economic sustainability assessment along the chemical life cycle, exploring possible options for the inclusion of this aspect.

The case studies were chosen according to the results of a stakeholder consultation held in 2021 (see Annex 2 of Caldeira et al, 2022a) and in alignment with relevant EC policies. Table 1 shows the group of chemicals considered for each case study, the application considered, and a brief description of the application of the chemicals.

Table 1. Group of chemicals considered for each case study, the application considered and a brief description of the focus of the case study

Group of chemicals	**Application**	**Short description of the case study**
Plasticisers (*non-phthalate*)	Food contact materials	Plasticisers used to soften PVC that is then used to produce gaskets to ensure the closure of glass jars.
Flame retardants (*halogen-free*)	Information and communications technology products	Flame retardants in reinforced polyamide applied in connectors.
Surfactants	Textiles processing	Enzymes used in the scouring of textiles to reduce the required amount of other chemicals.

The JRC applied the SSbD framework to a case study on non-phthalate plasticisers in food contact materials (FCM), i.e. chemicals already on the market. This case study was developed for illustrative purposes only. The results are presented in section 2, including a description of the case study (section 2.1), considerations on the (re)-design phase of the framework (section 2.2), the safety and sustainability assessment (section 2.3), and exploratory work on socio-economic assessment (section 2.4).

Additionally, the implementation of the framework was tested by companies for case studies on non-halogenated flame retardants in ICT (Information and communications technology) and on surfactants in scouring of textiles. These case studies and their preliminary results were presented during the 3rd stakeholder workshop held on the 9th and 10th February 2023 (relevant recordings are available here: day 1[4] and day 2[5]. A short description of them and feedback from the companies is presented in Section 3.

Lessons learned and challenges identified through the case study are presented in Section 4 and concluding remarks in Section 5.

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[4] https://www.youtube.com/watch?v=OcGydn2wyE0

[5] https://www.youtube.com/watch?v=SKTrtKrAr6Y

2 Case study 1: Plasticiser in food contact material

Food contact materials (FCM) such as those used in packaging, containers etc. are essential along the food production and consumption chain due to their role in preserving foodstuff from possible physical, chemical and microbiological hazards that can impact foodstuff nutritional quality and safety. A variety of materials including plastics, rubber, paper and metal, as well as additives such as plasticisers can be found in the packaging materials. Those materials may release hazardous substances into food, posing health concerns to the consumer. Therefore, safety must be proven on a case-by-case basis.

The use of plasticisers in packaging materials is widespread as they improve workability, extensibility and flexibility of a wide variety of polymers, such as polyvinyl chloride (PVC), polyethylene terephthalate (PET) etc., at the percentage of 10% up to 60% plasticisers by weight, to make them flexible and mouldable into different shapes. There are different types of plasticisers available on the market among which phthalates (in 2020, estimated market share in EU 50-60%), terephthalates, epoxies, and aliphatics are highly used.

The global plasticisers market is driven by the development of various industries such as packaging, the high request for flexible PVC used in various applications (e.g. coated fabrics, film and sheet coverings, consumer goods, medical devices, flooring etc.), as well as an increase in the use of non-phthalates and high molecular weight phthalate plasticisers.

In Europe, the use of certain phthalates is restricted in a wide range of products through several pieces of legislation (Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), Toys Directive, Restriction of Hazardous Substances in Electrical and Electronic Equipment (RoHS)) and highly controlled with very strict requirements in others (FCMs, Medical Devices). Therefore, the plasticiser sector is innovating and developing alternatives such as bio-plasticisers (e.g. epoxides, sebacates, succinic acid, citrates, glycerol esters, etc.) and in addition, the alternatives-to-phthalates (non-phthalate) segment in the plasticiser market is growing rapidly.

2.1 Case study description

This section describes the case study, including the plasticisers considered (section 2.1.1), the description of the system coverage of the assessment, and actors in the value chain (section 2.1.2)

2.1.1 Plasticisers under assessment

The case study on “non-phthalates plasticisers in Food Contact Material” was developed for existing plasticisers on the market and simulating a case in which a chemical of concern was identified and would need to be substituted. We then used the SSbD framework to assess the safety and sustainability performance of the chemical to be substituted and the alternatives, performing a comparative assessment.

The definition of the case study limits the scope to the application of plasticisers in FCM application. Therefore, relevant plasticisers are those that provide required technical property of softness and properties to be applied in FCM including the fulfilment in this case of the plastic FCM Regulation (EC, 2011a).

Di(2-ethyl hexyl) Phthalate (DEHP) was identified as the plasticiser of concern to be substituted and, therefore, used as “reference”. Alternative non-phthalate plasticisers were identified. The plasticiser of concern was compared with possible alternatives following what is currently done in alternative assessment.

For the selection of non-phthalate plasticisers already marketed alternatives have been selected following these criteria:

- As already existing alternatives, it is understood that they are feasible alternatives that provide similar technical properties as phthalates to PVC.
- As marketed alternatives, the information needed for the assessment of the applicability of the SSbD framework should be available.
- As marketed alternatives, they are authorised for FCM application.

From the different existing alternatives, the most used and recognised ones are selected (DEPA, 2014; Chemsec, 2019; European Plasticiser, 2023; CPSC, 2010).

Plasticisers considered in the case study

Reference

- Di(2-ethyl hexyl) Phthalate (**DEHP**)
- Among the phthalates, DEHP is the one of highest concern because of its classification as ‘Toxic for the Reproduction’ category 1B. In addition, it has been identified by the European Chemicals Agency (ECHA) as an endocrine disruptor (ED) for human health and the environment. Therefore, it has been identified as substance of very high concern (SVHC) under REACH. Moreover, together with several other phthalates, DEHP is listed in REACH Annex XIV, and thus it cannot be used unless an authorisation for the use is timely requested and obtained. In particular, it can be noted that the latest application date for the authorisation of the use of DEHP in FCM is 14 June 2023.

Alternatives

The non-phthalate plasticisers included in the case study (Table 2) are the following ones:

- Di(2-ethyl hexyl) terephthalate (**DEHT**) and di-isononyl cyclohexanoate (**DINCH**)
    - DINCH is the most used plasticiser alternative in Europe and DEHT in the US.
    - They are used as alternatives to phthalates in medical devices such as blood bags, in food contact materials such as artificial wine corks, in sports equipment and textile coatings, in wallpaper, paints and inks, adhesives and in cosmetics and toys.
    - Due to their low migration rate they are used in soft PVC.
- Di(2-ethyl hexyl) adipate (**DEHA**) and acetyl tributyl citrate (**ATBC**)
- Both are used in medical devices application as alternatives to phthalates.
- Defined by industry as the more commonly used monomeric plasticisers for food packaging PVC cling-films.
- Their intrinsic properties make them suitable alternatives to phthalates especially in the manufacture of food grade cling film.
- ATBC is used as a plasticiser in cosmetic products and in PVC applications.
- Epoxidised soybean oil (**ESBO**)
- As a representative plasticiser of vegetable origin.
- It is an important plasticiser in many formulations due to its dual role as plasticiser and stabiliser.
- It is used in glass jar gaskets and cling film for food wrapping.

Table 2. Identity information on the plasticisers used in the case study indicating the IUPAC (International Union for Pure and Applied Chemistry) name, CAS (Chemical Abstracts Service) number and EC (European Community) number

Common name	Acronym	IUPAC(2) name	CAS(3) number	EC(4) number	Molecular weight (g/mol)
Di-(2-ethyl hexyl) Phthalate	DEHP	Bis(2-ethylhexyl) benzene-1,2-dicarboxylate	117-81-7	204-211-0	390.57
Acetyl Tributyl citrate	ATBC	Tributyl 2-(acetyloxy)propane-1,2,3-tricarboxylate	77-90-7	201-067-0	402.48
Di(2-ethyl hexyl) adipate	DEHA	Bis(2-ethylhexyl) hexanedioate	103-23-1	203-090-1	370.57
Di (2-ethylhexyl) terephthalate	DEHT	Bis(2-ethylhexyl) benzene-1,4-dicarboxylate	6422-86-2	229-176-9	390.56
Di(isononyl) cyclohexane-1,2-dicarboxylate	DINCH	Bis(7-methyloctyl) cyclohexane-1,2-dicarboxylate	166412-78-8	605-439-7	424.67
Epoxidized soybean oil	ESBO	-	8013-07-8	232-391-0	975.41(1)

(1) Average molecular weight; (2) International Union of Pure and Applied Chemistry, (3) Chemical Abstract Service, (4) European Community

In order to apply the framework, a **specific use** needs to be defined which implied the selection of a product in which the plasticiser is used. After consultation with several stakeholders and based on their feedback on current market application and data availability, the **selected product is a sealing gasket** made of a plastic liner with elastomeric properties (e.g. plastisol) placed below the metal cap in glass jars (see Figure 1). Detailed information on the gasket is provided in Annex 1.

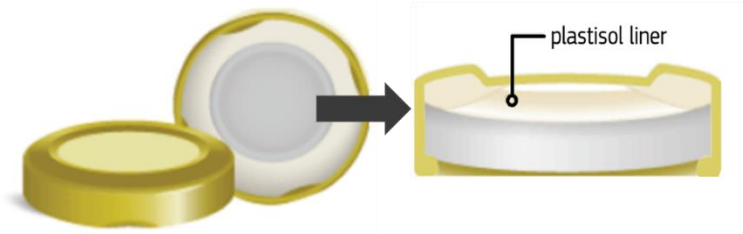


Figure 1. Product (gasket - plastisol liner) in which the plasticiser is used (image adapted from sks-bottle.com)

2.1.2 System description, coverage of the assessment, and actors in the value chain

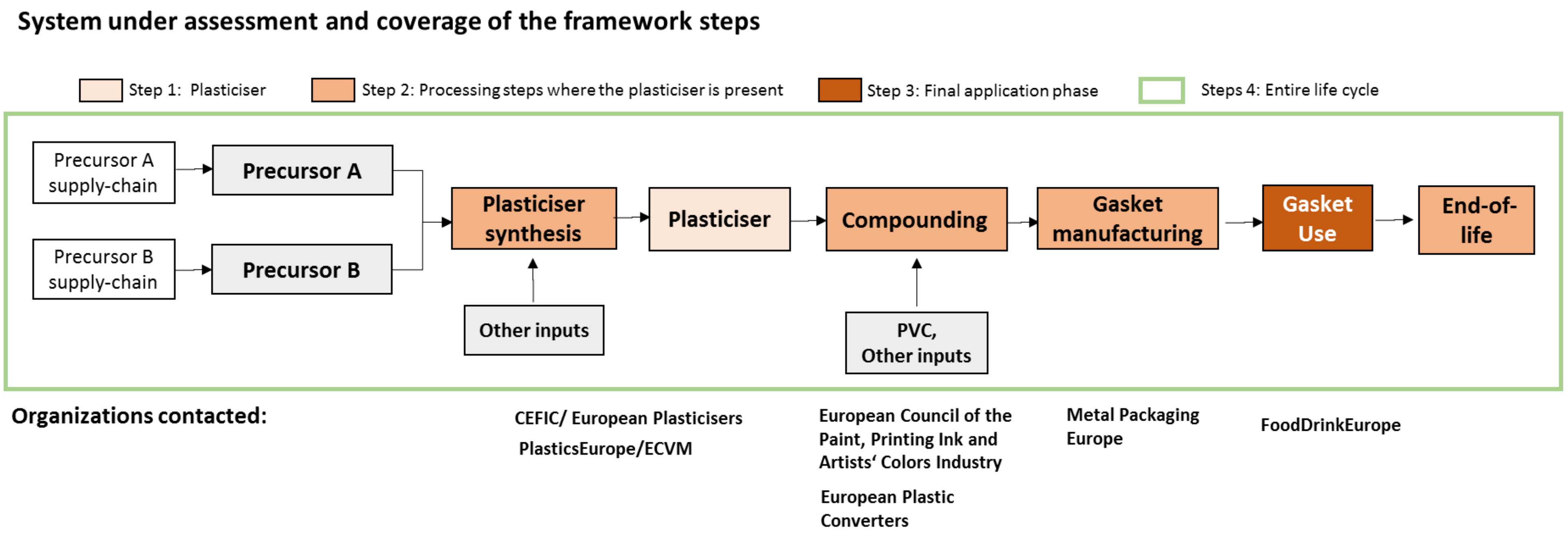
The SSbD concept adopts a life cycle perspective and therefore the entire life cycle of the plasticiser should be considered. Figure 2 illustrates a general description of the system under assessment, as well as what is covered in each of the assessment steps. The system includes the production of precursors used to produce the plasticiser (as well as other inputs required), mixing the plasticiser with PVC and other additives to produce the plastisol that will be applied as a plastic liner (gasket) inside the metal cap to enable the sealing of glass jars. The system also considers the end-of-life of the gasket.

When developing the case study, to learn about the system under assessment and engage with companies that could provide primary data, the JRC contacted several associations representing the different sectors of the value chain (Figure 2). To obtain information on plasticisers' production, meetings have been organised with the *European Plasticisers,* a sector group of the *European Chemical Industry Council (CEFIC)*, and with companies associated with *ChemSec* (International Chemical Secretariat). This exchange provided information on the more appropriate FCM application (i.e. product) for the plasticisers and four companies volunteered to provide data for the JRC study.

To obtain information on the plastisol formulation, the JRC met with the *European Council of the Paint, Printing Ink and Artists' Colours Industry (CEPE),* as well as with the *European Plastic Converters (EuPc)* that provided feedback on the formulations under assessment. The sector formulating and applying the plastisol in this value chain is normally the sector that manufactures the metal caps represented by *MetalPackagingEurope*, with whom the JRC also met. It was not possible to obtain specific information for this process. However, some support was received from one member company.

Finally, to learn about the requirements to use the plasticiser in FCM, the JRC met with the association *Food Drink Europe* that illustrated in which "use" conditions the gasket would need to be tested, the main features of the testing and what is currently required in the FCM legislation

Figure 2. Description of the case study system and sources of information for each step



These exchanges highlighted very well the complexity of the chemicals/materials-products value chains and the challenges to obtain all the information needed for the application of the SSbD framework. This information is sometimes sector/company specific and therefore not publicly available. Given that the chemicals'/materials' value chains are long and involve many players, this can be considered a major challenge for the application of the SSbD framework. Moreover, very often the producer of the chemical/material, in this case the plasticiser, does not have all the information regarding the downstream processes in which the chemical will be used.

2.1.2.1 Plasticisers production

2.1.2.1.1 Di(2-ethyl hexyl) Phthalate – DEHP

Di-(2-ethyl hexyl) Phthalate (DEHP) is an organic compound, liquid at room temperature, transparent and soluble in oil. It is the diester of the phthalic acid and 2-ethylhexanol. It is one of the most common plasticisers in the global market, especially for PVC application.

The production of DEHP is done through an esterification process in two steps. The first reaction between the phthalic anhydride and the 2-ethylhexanol gives the ester mono-2-ethylhexyl phthalate and water as a by-product. The equilibrium of this reaction leads to complete conversion of the reactants. The second reaction is the formation of the DEHP, to push the equilibrium of this reaction towards the product as much as possible, the water is eliminated before the second reaction by distillation and the reactor works with an excess of alcohol.

The reactors operate at medium (140-160°C) or high temperatures (200-250°C) depending on the catalyst used. After the second reactor, the unreacted alcohol is recovered with a distillation column and fed back to the reactors (COWI et al., 2009).

2.1.2.1.2 Acetyl tributyl citrate (ATBC)

Citric acid plasticisers are considered the first choice as nontoxic and safe plasticisers in many applications such as food packaging, medical equipment, and toys for children (Jia et al., 2018). Its basic raw material of, citric acid, is obtained via fermentation process of organic biomass.

ATBC is partly a bio-based plasticiser, due to the presence of citric acid. It has various uses: as plasticiser in food packaging film, for biomedical and biodegradable materials (Fang et al., 2018).

ATBC is produced via a two-step reaction. In the first step, Tributyl Citrate (TBC) is produced by the reaction of citric acid and n-butanol at the presence of a catalyst (H_2SO_4) (Osorio-Pascuas et al., 2015). The reaction conditions are 120°C of reaction temperature, and 0.5–1.5% of catalyst concentration.

Afterwards, ATBC can be produced through direct esterification of TBC with acetic acid (Sakakura, Nakagawa, et al., 2007) or through acetylation with acetic anhydride (Sakakura, Kawajiri, et al., 2007). The latter synthesis route produces acetic acid as a by-product and it was used to model the reaction.

The acetic acid produced was considered as part of the wastewater sent to treatment, since its low concentration makes it difficult to recover it.

2.1.2.1.3 Di(2-ethyl hexyl) Adipate (DEHA)

DEHA is one of the esters of adipic acid. It has a good oxidation stability, low toxicity and volatility, high biodegradability and viscosity (Acciaretti, Pasquale, 2020). All these properties make it widely used in many applications: paint stripper, fragrance, lubricant, food packaging and plasticiser (Chaibakhsh et al., 2009). As plasticiser, it provides various properties for PVC: flexibility, elasticity and workability; it is also less sensitive to temperature changes, because it is more fluid at low temperatures and less volatile at high temperatures (Gryglewicz Oko, 2005).

Classical DEHA production is based on Fischer esterification of adipic acid and monohydric alcohols (2-ethyl hexanol), using acid chemical catalysts as methanesulfonic acid, cation-exchange resins and modified heteropoly acids (Acciaretti Pasquale, 2020).

2.1.2.1.4 Di(2-ethyl hexyl) Terephthalate (DEHT)

The DEHT is produced by the esterification of terephthalic acid and 2-ethylhexanol. Terephthalates are not ortho-phthalates, but they have a similar chemical structure and technical properties, so they are used in some applications to substitute the corresponding phthalate.

2.1.2.1.5 Di(isononyl) cyclohexanoate (DINCH)

The hydrogenation process is used on several phthalates' derivatives, aiming to convert them into the corresponding cyclohexanoates to improve their intrinsic safety. In the case of DINCH, this is achieved through the catalytic hydrogenation of the Di-isononyl phthalate (DINP). The details of the process are not publicly available and can be inferred partially by patents (Brunner et al., 2001) and by similarities with other hydrogenation processes.

The manufacturing of DINP and its precursors is similar to the DEHP one. The isononyl alcohol is manufactured through the hydroformylation of C-8 alkanes, which can be produced from C4 raffinate through butadiene separation and dimerisation, or via the polygas process producing a mixture of C7-9 alkanes. Then, the alcohol reacts with phthalic anhydride to produce DINP. An LCA of the DINP has been performed by 'European Plasticisers' and it is used for the modelling of DINCH in the present study (ECPI, 2015).

2.1.2.1.6 Epoxidised soybean oil (ESBO)

Vegetable oils may be a promising route to renewable plasticisers since they are biodegradable and have low toxicity. Different types of vegetable oils from different sources can be used: soybean, linseed, palm, castor bean. Among the different vegetable oils, Epoxidized soybean oil (ESBO) is the most common oleochemical used for PVC compounding. Nowadays, its global production is about 240000 t/year, with a European production of 90000 t/year.

ESBO and also other epoxidised vegetable oils are used as stabilisers and plasticisers for PVC, to improve its flexibility and elasticity.

The production process involves soybean oil, an aqueous solution containing hydrogen peroxide (H_2O_2) and formic or acetic acid and sulfuric or phosphoric acid (Alhanish Abu Ghalia, 2021). The organic acid reacts with hydrogen peroxide to form a peroxy acid, which can diffuse into the oil and epoxidise it. This reaction regenerates the initial organic acid which then acts similarly to a catalyst. The reaction, normally, requires 6-10 hours to be completed keeping the temperature between 60 and 75°C.

The reaction is highly exothermic ($\Delta H = -55$ kcal/mol for each double bond), which requires to slowly add the mixture of H_2O_2 and formic or acetic acid to the mixture of oil and acid catalyst, to avoid a steep increase in temperature (Alhanish Abu Ghalia, 2021). For this reason, the reaction takes place in pulse-fed-batch or fed-batch reactors in industry, by gradually adding the oxidants to the oil that allows to control the reaction temperature. The reaction is followed by hydrogen peroxide decomposition step, by using sodium hydroxide and a neutralization step (Kralisch et al., 2012). Afterwards, the aqueous phase is separated and the product is washed and filtered.

2.1.2.2 Compounding: Plastisol Production

Plastisol is a colloidal suspension of small dispersed PVC particles, with a diameter of 0.1–5 μm, in a liquid plasticiser matrix (Saeki Emura, 2002). A description of its production steps and operation conditions is reported hereunder.

In the plastisol production, the PVC used is an emulsified PVC (E-PVC) (Saeki Emura, 2002). E-PVC and the other additives (e.g. stabilisers, fillers, pigments, etc.), which are reported in Table 3, are all added into a blender, named Banbury mixer, along with a plasticiser, by forming a paste (Yalcin, 2015). During this process that can last about 60 min, the intensive mixing applied can cause a temperature increase. To avoid this issue of heating-up to 50-75°C, the blender is cooled with an external jacket fed with water (Graham, 1973).

The material formed by this step is a paste, named plastisol. It has the properties of a visco-elastic liquid at room temperature.

In most cases, plastisols are de-aerated after mixing and stored at controlled temperatures, preferably below 23°C, to prevent heat-induced viscosity increase and other changes in their desired rheology caused by aging (Wilkes et al., 2006).

When combined with PVC, plasticisers convert the rigid, intractable resins into workable compounds which can exhibit a wide range of properties depending on the type and concentration of plasticisers used (Arkema, 2013).

The selection of a plasticiser for the formulation of the plastisol requires the balancing of different qualities, properties and parameters of the plasticiser and of the PVC for the plastic material.

For the case study, among all the properties, there was a focus on the plasticiser efficiency (Shore A hardness) in softening the PVC for the gasket application. The Shore A Hardness for this application was identified to be between 60 and 80; 70 was chosen as the reference value.

Based on this, the substitution factor shown in Table 3 represents the quantity of a plasticiser needed to soften the PVC at a given level, compared to the quantity of a reference plasticiser (DEHP).

Table 3. Summary of the composition of the gasket for each of the selected plasticisers

Component of the gasket	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Substitution factor	1	1.06	0.93	1.03	1.09	1.1
Plasticiser	35.8%	37.2%	34%	36.5%	37.8%	38.0%
PVC	47.8%	46.8%	49%	47.2%	46.3%	46.1%
Blowing Agent (sodium bicarbonate)	0.6%	0.6%	1%	0.6%	0.6%	0.6%
Stabiliser (zinc stearate)	1.2%	1.2%	1%	1.2%	1.2%	1.2%
Lubricant (stearic acid)	4.1%	4.0%	4%	4.0%	3.9%	3.9%
Pigment (TiO_2)	0.6%	0.6%	1%	0.6%	0.6%	0.6%
Filler (calcium carbonate)	10.0%	9.8%	10%	9.9%	9.7%	9.7%

2.1.2.3 Gasket manufacturing

The gasket production involves the following steps: i) pre-heating the plastisol, then ii) the plastisol is injected into the article (i.e. metal cap) and finally iii) it becomes solid when cured in the oven and the gasket is formed.

During the pre-heating, the plastisol produced in the previous stage (the compounding step) is heated up to 70-110°C at which the gelation process happens: the adsorption of plasticiser by PVC particles takes place because of an increase of the temperature and/or a drastic ageing (Marcilla et al., 2017). Once the pre-heating step is completed, plastisol is then injected into the metal cap and it is casted in the final step. Data are not available for this process, therefore the energy consumption for injection was estimated as part of the heating of the material, since the energy consumed in injecting a viscous liquid is mostly transformed in heat and therefore in temperature increase of the material.

The final step is the curing of the material by passing through an oven (Graham, 1973). In this step fusion mechanism takes place, thus the PVC particles and the plasticiser melt together to form a homogeneous material with the desired mechanical properties when it is cooled down (Marcilla et al., 2017). Temperature varies from 150°C to 190°C (Graham, 1973). The energy requirement for this step, has been estimated from a previous work, in which a similar mixture is cured in a high-velocity hot-air tunnel oven (Boluk et al., 1990).

2.1.2.4 Gasket use

The use phase of the gasket starts after the curing of the cap, when it is ready for the subsequent use in the food packaging process. In the canning process, the jar is closed mechanically and thermally treated to preserve the content. Since these operations are done for the purpose of preserving the food, their environmental burden shall be accounted in the system boundaries of the food.

However, some aspects of the use phase may be relevant for the assessment at step 3, such as:

- Heat-treatment: what kind of thermal treatment is used and for how long, considering that shelf-stable foods are subject to sterilising treatment to eliminate all spores and vegetative bacteria able to grow in the food, so that they can be stored at ambient temperature while sealed (Koutsoumanis et al., 2021).
- Time: based on the study of McCombie et al. (2012), most of the sampled products showed significant plasticiser migration from one to four years from the end of their shelf-life. Furthermore, compliance of the product should be tested at the end of the shelf life. Therefore, three scenarios can be considered (or a combination of the first with the other two):
  - For 6, 12, 24, 36 or 48 months unopened glass jar at ambient temperature (to be selected in the step 3);
  - 7, 10 days in the fridge (4°C) as opened package;
  - 2, 4 months in the freezer (-18°C) opened glass jar.
- Other relevant properties of the food such as alcohol content, free fat content and pH.

2.1.2.5 Gasket End-of-life

The end-of-life of the gasket is linked to the end-of-life of the cap which can be considered a single use packaging. It is assumed that all the caps are part of the municipal waste flow.

2.2 Design (or re-design)

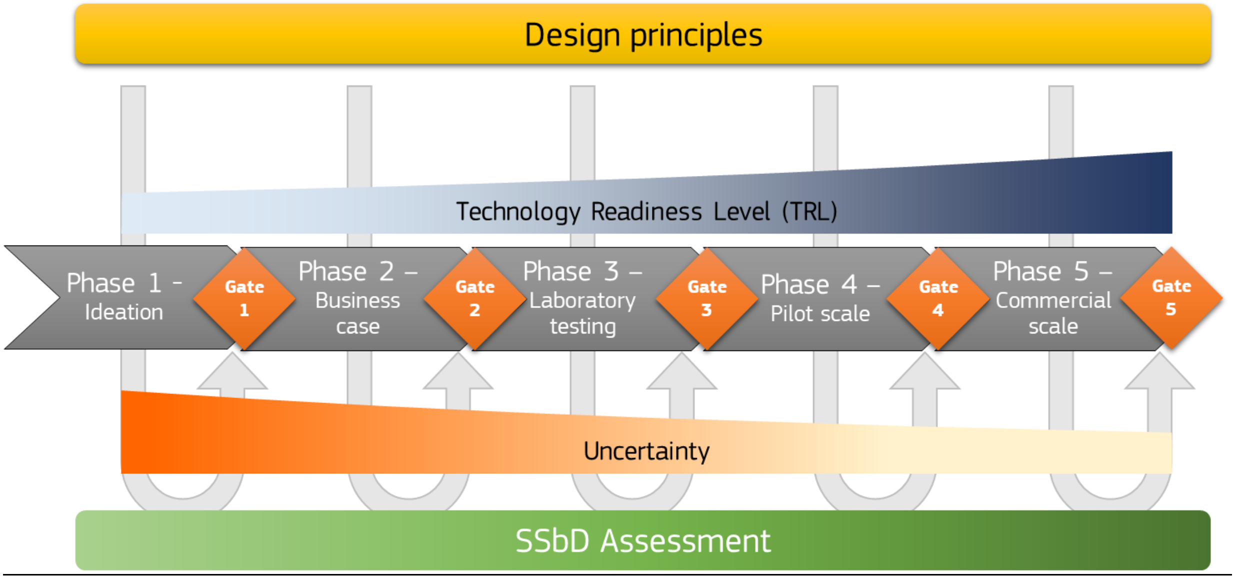
As mentioned in section 1.4, the SSbD framework considers two phases 1) Design (or re-design) phase in which guiding design principles (reported in Table 4) are proposed to support the development of safe and sustainable chemicals and materials, and 2) Safety and sustainability assessment phase in which the safety and sustainability of the chemical(s) or material(s) in question are assessed. These two phases are iterative along the innovation process, meaning a safety and sustainability assessment is performed since the early stages of development (Figure 3)

As an example of possible integration between the SSbD and the innovation process, one of the most used approaches in this context is a phase-gate approach (Cooper, 2010). This iterative approach encompasses several iterations of a development phase by parallel assessments of alternatives followed by a decision moment (i.e. gate), in which the alternatives are screened out using a set of criteria relevant for that phase. A general scheme of this approach is shown in Figure 3. The SSbD assessment can be integrated to this method by using design principles along the development phase, and performing the SSbD assessment in the gate to validate/adjust the design, accordingly. However, the SSbD assessment needs to be adapted reflecting the specific data availability throughout the Technology Readiness Levels (TRLs) of the innovative process, which influence the overall uncertainty of the SSbD assessment.

Table 4. SSbD design principles as defined in Caldeira et al. (2022b)

SSbD principle	Definition
SSbD1 Material efficiency	Pursuing the incorporation of all the chemicals/materials used in a process into the final product or full recovery inside the process, thereby reducing the use of raw materials and the generation of waste.
SSbD2 Minimise the use of hazardous chemicals/materials	Preserve functionality of products while reducing or completely avoid using hazardous chemicals/materials where possible.
SSbD3 Design for energy efficiency	Minimise the overall energy used to produce a chemical/material in the manufacturing process and/or along the supply chain.
SSbD4 Use renewable sources	Target resource conservation, either via resource closed loops or using renewable material/ secondary material and energy sources.
SSbD5 Prevent and avoid hazardous emissions	Apply technologies to minimise and/or to avoid hazardous emissions or pollutants in the environment.
SSbD6 Reduce exposure to hazardous substances	Eliminate exposure to chemical hazards from processes as much as possible. Substances which require a high degree of risk management should not be used and the best technology should be used to avoid exposure along all the life cycle stages.
SSbD7 Design for end-of-life	Design chemicals/materials in a way that, once they have fulfilled their function, they break down into products that do not pose any risk to the environment/humans. Design for preventing the hindrance of reuse, waste collection, sorting and recycling/upcycling.
SSbD8 Consider the whole life cycle	Apply the other design principles thinking through the entire life cycle, from supply-chain of raw materials to the end-of-life in the final product

Figure 3. An example of linking between the innovation process, the design principles and the SSbD assessment



2.3 Safety and Sustainability assessment

2.3.1 Step 1 Hazard assessment of the chemical/material

2.3.1.1 Goal and scope

The question that needs to be answered in Step 1 relates to the 'hazard level' in which the chemical/material falls under, when applying the SSbD criteria for the hazard properties.

The SSbD criteria are based on the Classification, Labelling and Packaging (CLP) Regulation ((EC) No 1272/2008). CLP (EU, 2008) harmonises criteria to classify chemicals that are hazardous according to their intrinsic physico-chemical, toxicological and ecotoxicological properties.

Therefore, relevant available information for the purposes of determining whether the chemical entails a physical, health or environmental hazard as set out in Annex I of the CLP has to be gathered and assessed. When relevant information on a chemical/material meets the classification criteria in CLP, the hazards are identified by assigning a certain hazard class and category. The hazard classes in CLP cover physical, health, environmental and additional hazards.

Chemicals with certain hazard classes like CMRs and respiratory sensitiser are subject to harmonised classification procedure and when the process is concluded, if there is a decision on the harmonised classification, and Adaptation to Technical Progress updates Annex VI of the CLP with the entry of this harmonised classification.

2.3.1.2 Approach

This case was based on already existing chemicals in use, therefore, chemicals that have fulfilled the European regulatory requirements to be placed on the market (REACH, CLP and FCM). Information on the intrinsic properties of the chemicals that have been used to conclude on the hazard classification should therefore be available. It is understood that the process of gathering all available relevant information in order to draw a conclusion on the hazard classification according to the CLP criteria has already been done by industry experts for the compliance with the regulatory requirements.

The database of the European Chemicals Agency (ECHA) was chosen as the most transparent and comprehensive one among the ones searched.

The information on the chemicals' classification and concerning hazards was retrieved from the following data sources in the ECHA database:

- Harmonised classification in Annex VI of CLP from the Classification and Labelling inventory[6]
- Non-harmonised CLP Self-classification from REACH Registration Dossiers (Table 5)
- Additional hazards form the Candidate List of Substances of Very High Concern (SVHC)[7] and the Public Activities Coordination Tool-Risk Management Options Analysis (PACT RMOA).

Table 5. ECHA database links for the dossiers referring to the individual substances

Name	Acronym	EC	CAS	Link
Di (2-ethylhexyl) phthalate	DEHP	204-211-0	117-81-7	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15358/2/1
Acetyl tributyl citrate	ATBC	201-067-0	77-90-7	https://echa.europa.eu/registration-dossier/-/registered-dossier/13143/2/1
Di (2-ethylhexyl)adipate	DEHA	203-090-1	103-23-1	https://echa.europa.eu/registration-dossier/-/registered-dossier/15293/2/1
Di-ethylhexyl terephthalate	DEHT	229-176-9	6422-86-2	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15238/2/1
Di-isononyl cyclohexane dicarboxylate	DINCH	431-890-2	166412-78-8	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/16022
Epoxidised soybean oil	ESBO	232-391-0	8013-07-8	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15408

Data source: ECHA

2.3.1.3 Results

The information found is presented in Table 6, Table 7 and Table 8, respectively for the human, environmental, and physical hazard, respectively.

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[6] https://echa.europa.eu/information-on-chemicals/cl-inventory-database

[7] https://echa.europa.eu/candidate-list-table

Table 6. Classification of the plasticisers based on the ECHA database information – Human Health (HH) hazards

Plasticiser	**SVHC**	**CLP Annex VI entry**	**Data source**	**Human health hazards**													
				Carcinogenicity	Mutagenicity	Reproductive toxicity	ED (human)	Respiratory Sensitisation	STOT-RE	Skin sensitisation	Acute toxicity.: oral	Acute toxicity. Dermal	Acute toxicity Inhalation	Skin corrosion/irritation.	Eye damage/irritation	Aspiration hazard	STOT-SE
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	**NC**	**NC**	**1B**	**POS**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
ATBC	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**MISS**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DEHA	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DEHT	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**MISS**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DINCH	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**MISS**	**NC**	**NC**	**NC**	**NC**	**MISS**	**NC**	**NC**	**MISS**	**NC**
ESBO	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**MISS**	**MISS**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**MISS**	**NC**

XXX	Classified XXX according to CLP criteria
NC	Not classified according to CLP criteria
MISS	Data missing

XXX	No CLP hazard classes
POS	Confirmed SVHC
NEG	No SVHC

SVHC= Substance of very high concern; ED= Endocrine Disruptor; STOT-RE= Specific target organ toxicity - repeated exposure; STOT-SE= Specific target organ toxicity - single exposure

Table 7. Classification of the plasticisers based on the ECHA database information – Environmental hazards

Plasticiser	SVHC	CLP Annex VI entry	Data source	Environmental hazard					
				PBT/vPvB	PMT/vPvM	ED (environment)	Ozone	Chronic aquatic toxicity	Acute aquatic toxicity
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	POS	MISS	POS	MISS	NC	NC
ATBC	NO	NO	ECHA Registration	NEG	MISS	MISS	MISS	NC	NC
DEHA	NO	NO	ECHA Registration	NEG	MISS	MISS	MISS	NC	NC
DEHT	NO	NO	ECHA Registration	NEG	MISS	NEG	MISS	NC	NC
DINCH	NO	NO	ECHA Registration	NEG	MISS	MISS	NC	NC	NC
ESBO	NO	NO	ECHA Registration	NEG	MISS	MISS	MISS	NC	NC

NC	Not classified according to CLP criteria
MISS	Data missing

XXX	No CLP hazard classes
POS	Confirmed SVHC
NEG	No SVHC

Table 8. Classification of the plasticisers based on the ECHA database information – Physical hazards

Plasticiser	SVHC	CLP Annex VI entry	Data source	Physical hazards											
				Explosives	Flammable	Aerosols	Oxidizing	Gases under pressure	Self-reactive	Pyrophoric liquids, solids	Self-heating	Emits flammable gas	Organic peroxides	Corrosivity	Desensitized explosives
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	MISS	MISS
ATBC	NO	NO	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	MISS	MISS
DEHA	NO	NO	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC
DEHT	NO	NO	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	MISS
DINCH	NO	NO	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC
ESBO	NO	NO	ECHA Registration	NC	NC	NC	NC	NC	NC	NC	NC	NC	NC	MISS	MISS

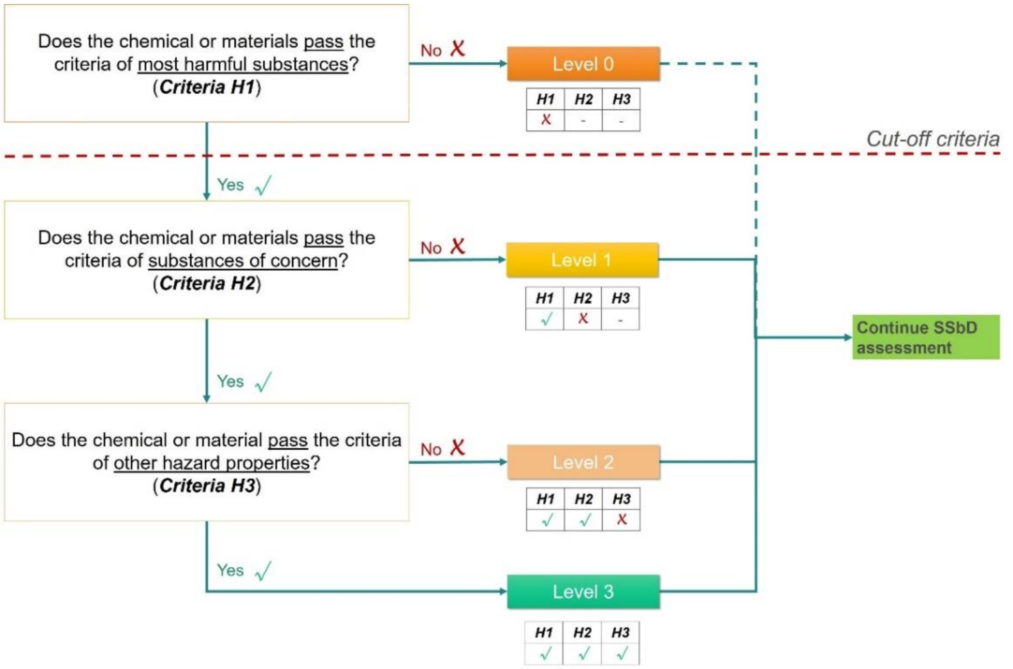
NC	Not classified according to CLP criteria
MISS	Data missing

2.3.1.4 Discussion

Only DEHP has a Harmonised Classification in Annex VI of CLP, and it is as well the only chemical identified by the ECHA Member State Committee (MSC) as ED (Endocrine Disruptor) for both the HH (Human Health) and the ENV (Environment).

None of the alternatives has a harmonised classification. However, according to the SSbD criteria, in order to pass the Step 1 assessment, all the information should be available. And, as it can be seen from the table, data is missing to conclude about some hazard classes. Therefore, none of the plasticisers could be considered safe according to the SSbD criteria for Step 1 (Figure 4) due to the non-completeness of the hazard data.

Figure 4. Workflow relevant to Step 1 of the SSbD framework



It has to be understood, however, that the lack of data may have a justification like:

- The data requirements under REACH are linked to the volumes of chemicals that are placed on the market per year. And in some cases, the data missing in the ECHA database might be due to this fact. It is not the case of the plasticisers assessed in this case study. They all have been registered for the higher tonnage band.

  However, the SSbD does not consider this aspect in its assessment and all the needed information for classification purposes according to the SSbD criteria should be available/generated in order to assess the chemical/material hazard profile in its integrity. To achieve this, an Integrated Approach for Testing and Assessment (IATA) should be followed in order to gather all available information for assessing and weighing and draw a conclusion, and generate new data using New Approach Methodologies (NAMs) (see additional information in Annex 2).

Data needed to conclude on some of the hazard classes is not required for REACH registration. For example, hazardous to the ozone layer or corrosivity to metals.

- Some of the hazard classes considered in the SSbD criteria for Step 1 were not hazard classes under CLP until very recently: ED (Endocrine Disruptor), PBT (Persistent Bioaccumulative and Toxic), PMT (Persistent Mobile and Toxic).

The legislative proposal of the European Commission setting the criteria for the identification of these hazard classes under the CLP Regulation was published in the Official Journal of the European Union on the 31st of March 2023. The delegated act (EU, 2023) entered into force the 19th of April.

Until now, the process to assess and identify them has been through the REACH authorisation process as of Equivalent level of concern (ELoC) having probable serious effects to the human health and/or the environment (Article 57(f)). Member States or ECHA (at the request of the European Commission) are the responsible of initiating this process if a concern exists with regards to these hazard properties.

For DEHP the outcome of the assessment has been the identification as ED both for the HH and the ENV.

DEHA and DINCH have also gone through the assessment as ED for the HH and the outcome has been negative, meaning that they have not been identified as ED for the HH.

The rest of the plasticisers have not been proposed for the assessment, understanding that no concern has been raised with regards to these properties.

As in previous points, if available data is insufficient or no data is available at all to reach a conclusion on the above-mentioned hazard properties, this data should be gathered or generated.

- Data missing can be due to data waiving. In this case, a clear justification should be provided.

  Data generation for some endpoints is not feasible (e.g., due to phys/chem properties), not required (e.g., because exposure route unrealistic) or there are no test methods (e.g., respiratory sense).

  This can be applied for instance to the Acute toxicity by inhalation hazard class. For substances with a vapour pressure below 0.01 Pa, an acute inhalation study is not required under REACH.

Data missing from some of the hazard classes in Table 6, Table 7 and Table 8 could be justified as follows:

Human health hazards Table 6:

- Respiratory sensitisers. Substances shall be classified as respiratory sensitisers (Category 1) if there is evidence in humans that the substance can lead to specific respiratory hypersensitivity and/or if there are positive results from an appropriate animal test.

  There are no standardised tests for respiratory sensitisation, and this is not a standard data requirement. Unless there are reports of the substance inducing allergic asthma, no data is submitted for this endpoint.
- Acute toxicity by inhalation hazard class. For substances with a vapour pressure below 0.01 Pa, an acute inhalation study is not required under REACH.
- Aspiration toxicity hazards. A substance is classified in Category 1 based on reliable and good quality human evidence or if it is a hydrocarbon and has a kinematic viscosity of 20.5 mm^2/s or less, measured at 40°C.

  Only the dynamic viscosity is provided in the Registration Dossiers. The kinematic viscosity (mm^2/s) could be calculated by dividing the dynamic viscosity (mPa s) by the density (g/cm^3). Thus, for substances with densities around 1 g/cm^3, the values for dynamic and kinematic viscosity are similar. But since the plasticisers are carboxylic acid esters and not hydrocarbons, the aspiration toxicity category does not apply.

Environmental hazards Table 7:

- Hazardous to the Ozone Layer. A substance is classified as Hazardous to the Ozone Layer only if there is available evidence concerning its properties and its predicted or observed environmental fate and behaviour that may present a danger to the structure and/or the functioning of the stratospheric ozone layer.

  No testing required. If the substance is not on the list of ozone-depleting substances (Annex I to Regulation 1005/2009), the substance will not be classified as hazardous to the ozone layer. Also, none of the plasticisers has a halocarbon fraction in its structure which is a prerequisite for ozone-depleting properties.

Physical hazards Table 8:

- Corrosivity to metals. Corrosion rate on either steel or aluminium surfaces exceeding 6.25 mm per year at a test temperature of 55°C when tested on both materials.

  Normally, the waiver for this endpoint comes from industrial experience with storing or handling the substance in metal containers. In addition, it could be assumed that if the plasticiser is not corrosive to the skin might not be corrosive to metals.

- Desensitized explosives. It is only applicable for explosives. None of the plasticisers is classified as explosive.

If these justifications are considered to justify the missing data, the classification of the plasticisers is as presented in Table 9, Table 10 and Table 11, respectively for the human, environmental, and physical hazard.

Table 9. Classification of the plasticisers. Human health hazards

Plasticiser	SVHC	CLP Annex VI entry	Data source	Human health hazards													
				Carcinogenicity	Mutagenicity	Reproductive toxicity	ED (human)	Respiratory. Sensitisation	STOT-RE	Skin sensitisation	Acute toxicity: oral	Acute toxicity Dermal	Acute toxicity Inhalation	Skin corrosion./irritation	Eye damage/irritation	Aspiration hazard	STOT-SE
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	**NC**	**NC**	**1B**	**POS**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
ATBC	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NP**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DEHA	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DEHT	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NP**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
DINCH	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NEG**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**
ESBO	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NP**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**

XXX	Classified XXX according to CLP criteria
NC	Not classified according to CLP criteria

XXX	No CLP hazard classes
POS	Confirmed SVHC
NEG	No SVHC
NP	Not identified as SVHC

SVHC= Substance of very high concern; ED= Endocrine Disruptor; STOT-RE= Specific target organ toxicity - repeated exposure; STOT-SE= Specific target organ toxicity - single exposure

Table 10. Classification of the plasticisers. Environmental hazards

Plasticiser	SVHC	CLP Annex VI entry	Data source	Environmental hazard					
				PBT/vPvB	PMT/vPvM	ED (environment)	Ozone	Chronic aquatic toxicity	Acute aquatic toxicity
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	POS	NP	POS	NC	NC	NC
ATBC	NO	NO	ECHA Registration	NEG	NP	NP	NC	NC	NC
DEHA	NO	NO	ECHA Registration	NEG	NP	NP	NC	NC	NC
DEHT	NO	NO	ECHA Registration	NEG	NP	NP	NC	NC	NC
DINCH	NO	NO	ECHA Registration	NEG	NP	NP	NC	NC	NC
ESBO	NO	NO	ECHA Registration	NEG	NP	NP	NC	NC	NC

NC	Not classified according to CLP criteria

POS	Identified, assessed and agreed SVHC by the ECHA MSC
NEG	Identified, assessed and agreed No SVHC by ECHA MSC
NP	Not identified as SVHC

PBT= Persistent Bioaccumulative and Toxic; vPvB= very persistent and very bioaccumulative; PMT= Persistent Mobile and Toxic; vPvM= very persistent and very mobile

Table 11. Classification of the plasticisers. Physical hazards

Plasticiser	SVHC	CLP Annex VI entry	Data source	Physical hazards											
				Explosives	Flammable	Aerosols	Oxidizing	Gases under pressure	Self-reactive	Pyrophoric liquids, solids	Self-heating	Emits flammable gas	Organic peroxides	Corrosivity	Desensitized explosives
DEHP	Repr. 1B and ED (HH and ENV)	Repr. 1B	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**
ATBC	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**
DEHA	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**
DEHT	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**
DINCH	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**
ESBO	NO	NO	ECHA Registration	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NC**	**NA**

NC	Not classified according to CLP criteria
NA	Not applicable

Following the workflow shown in Figure 4, Table 12 shows the outcome of the SSbD scoring for the plasticisers after the adjustment of the results due to the lack of data. DEHP is classified as Reproductive toxicity Category 1B and in addition has been identified as Endocrine Disruptor for Human Health and for the Environment. Therefore, it does not pass the H1 criteria of the Step 1 of the SSbD and scores 0 following the workflow. The alternative plasticisers are not classified for any of the hazard classes included in the SSbD criteria and therefore pass criteria H2 and H3 and score 3 in the SSbD assessment for Step 1.

Table 12. SSbD scoring for Step 1

Plasticiser	**SSbD Score Step 1**
DEHP	0
ATBC	3
DEHA	3
DEHT	3
DINCH	3
ESBO	3

2.3.1.5 Conclusions for step 1

After looking for justification of the missing data, there are still data gaps to draw a conclusion on some CLP hazard classes (hazard criteria). In order to be able to conclude on the hazard classification of the plasticisers, data need to be generated for the new hazard classes under the CLP (ED, PBT, and PMT).

Additional data sources could be used to fill in the data gaps and conclude in certain hazard classes. However, one should be aware that alternative data sources could use different criteria and different categories to those in CLP to classify the hazard profile. One also should take into consideration, especially if the focus is a comparative assessment among different chemicals, like in this case study, that not all the databases provide this information for all the chemicals under assessment. Therefore, consistency should also be considered when filling these data gaps.

In order to ensure consistency, one could generate data using Quantitative Structure Activity Relationships (QSAR) models. These models should be seen as screening-level tools and should not be used if acceptable measured values are available. In these cases, one should ensure applicability of the models and the reliability of the data generated.

Two examples are presented below to illustrate these considerations.

An illustrative example is provided Table 13 where different data sources/lists for identifying ED properties have been screened:

- DEDuCT: Database of Endocrine Disrupting Chemicals and their Toxicity Profiles[8]
- ECHA SVHC Database
- EDslist: Endocrine Disruptor Lists[9]
- TEDX List: The Endocrine Disruption Exchange list[10]

On one hand, none of them classify ED properties following the SSbD criteria where different categories are considered for both the HH and the ENV. The recently published new criteria for EDs under the CLP is expected to improve the availability of data/information and a harmonised classification. On the other hand, none of them

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[8] https://cb.imsc.res.in/deduct/

[9] https://edlists.org

[10] https://endocrinedisruption.org/interactive-tools/tedx-list-of-potential-endocrine-disruptors/search-the-tedx-list

provide the same data/classification for all the plasticisers being assessed in this case study, where consistency is key.

Table 13. Screening exercise for Endocrine Disruption classification/listing of plasticisers

Plasticiser	DEDuCT	ECHA	EDs list	TEDXlist
DEHP	Category II	ED HH, ED ENV	list I: SVHC	Potential ED
ATBC	Category IV	No ED	In none of the lists	NO data
DEHA	Category III	No ED	In none of the lists	Potential ED
DEHT	No data	No ED	In none of the lists	NO data
DINCH	Category III	No ED	In none of the lists	NO data
ESBO	No data	Not assessed	In none of the lists	NO data

(DEDuCT=Database of Endocrine Disrupting Chemicals and their Toxicity Profiles; ECHA = European Chemical Agency; EDslist = Endocrine Disruptor Lists; TEDX List: The Endocrine Disruption Exchange list)

Table 14 is another example of gathering data in this case using Quantitative Structure Activity Relationships (QSAR) models. It summarises the values of the partition coefficient octanol-water (Kow) for the plasticisers using several publicly available and known QSAR tools and models.

The partition coefficient octanol-water is an important parameter in the safety assessment of a chemical/material as provides information about its distribution between aqueous and organic media. And it is also used to estimate other physical properties and toxicities.

Table 14. LogKow estimation for the plasticisers using different commercial QSAR (Quantitative Structure–Activity Relationship) tools

Source	Model	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
VEGA[11]	**LogP model (Meylan-KOWWIN)-assessment 1.1.5**	4.29 (LOW reliability)	8.12 (MODERATE reliability)	8.39 (MODERATE reliability)	8.39 (MODERATE reliability)	9.82 (LOW reliability)	14.84 (LOW reliability)
	LogP model (MLogP)-assessment	2.67 (LOW reliability)	4.74 (LOW reliability)	5.43 (LOW reliability)	5.43 (LOW reliability)	5.18 (LOW reliability)	5.21 (LOW reliability)
	LogP model (ALogP)-assessment	3.72 (LOW reliability)	7.04 (MODERATE reliability)	7.57 (GOOD reliability)	7.57 (GOOD reliability)	8.37 (LOW reliability)	13.26 (LOW reliability)
Danish EPA[12]	**EPI KOWWIN v1.68**	4.29	8.12	8.39	8.39	9.82	14.8
OECD QSAR[13]	**KOWWIN v1.67**	4.29	8.12	8.39	8.39	9.82	14.8
EPI SUITE[14]	**KOWWIN v1.69**	4.29	8.12	8.39	8.39	9.82	14.84
REACH Dossier	**Experimental**	4.86	8.94	7.50	8.94	10.00	>6.20

Most of these tools use the same QSAR model KOWWIN™ for the estimation of Kow. This model estimates the LogKow of chemicals using an atom/fragment contribution method. Therefore, it could be assumed that is a reliable model.

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[11] https://www.vegahub.eu/portfolio-item/vega-qsar/

[12] https://qsar.food.dtu.dk

[13] https://qsartoolbox.org

[14] https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

The Vega tool, in addition to the KOWWIN™ model the tool includes two additional models to estimate the same endpoint and that provide different results. And it also assesses the uncertainties of the models and integrates a level of reliability for the estimations. According to the tool the models present low reliability in the estimations for ATBC, DINCH and ESBO. In addition, if these values are compared with the experimental ones provided in the REACH Registration dossiers, it is evident that even those estimations with moderate and good reliability are not aligned.

These are some examples of the aspects that need to be considered when developing Integrated Testing Strategies to ensure that reliable data is generated without unnecessary animal studies. The degree of reliability and consistency will vary depending on the purpose of their use: screening, hazard identification, classification, filling specific data gaps.

2.3.2 Step 2 Human health and safety aspects in the chemical/material production and processing phase

2.3.2.1 Goal and scope

The goal of this step is to identify if the production and processing steps involving plasticisers pose any risk to the workers.

2.3.2.2 Approach

There are many different models and tools available for the exposure assessment to chemicals and materials. The Working Group Exposure Models of the European Regional Chapter of the International Society on Exposure Science (ISES Europe) provides an inventory that includes the most important exposure models and tools used in the EU (ISES Europe, 2022). The ISES Europe model inventory is a living document that is updated as new tools become available.

From the different methodologies and tools available, and following the same logic of Step 1, the CHEmical Safety Assessment and Reporting (Chesar) tool (ECHA, 2023a), developed by ECHA, has been chosen for the Tier 1[15] approach of the risk assessment in Step 2.

Chesar has a very user-friendly interface. It is publicly available in the dedicated ECHA website[16] and provides a lot of supporting information to perform the risk assessment.

Chesar facilitates the import of information from the hazard assessment conclusion in the REACH Registration Dossiers and relevant for the risk characterisation:

- Physico-chemical / fate properties
- Physico-chemical hazard
- Hazard conclusion and scope of assessment for:
    - Environment
    - Workers
    - Consumers

Moreover, it also provides the possibility to insert this input data manually.

For the case study, the information has been extracted from the publicly available information in the ECHA database and manually inserted in Chesar for each of the plasticisers (Annex 3), creating in that way a Chesar file for each of them.

In addition to the intrinsic properties of the chemical, information about the exposure must be known to perform the risk assessment. When measured data is not available, the uses of the chemical and the conditions under which

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[15] Screening level assessment using basic tools (e.g., simple exposure calculations, default values, conservative assumptions)

[16] https://chesar.echa.europa.eu/

the uses take place must be defined and the following type of information is required as a minimum by the Tier 1 screening tools:

How is the substance produced?

- Batch process;
- Continuous process.

Where is the substance produced?

- enclosed processes or plants;
- indoor controlled environment;
- indoor open sources;
- outdoor; etc.

What are the operational conditions?

- characteristics of the substance (physical state/dustiness/vapour pressure) and its concentration in a mixture or material under the operational conditions;
- duration and frequency of the activity;
- duration and frequency of exposure;
- temperature of the process; etc.

What are the risk management measures (RMM) in place?

- General ventilation;
- Local exhaust ventilation;
- General occupational safety and health (OSH) management systems (e.g., housekeeping, training…);
- personal protective equipment (PPE).

How is the substance used?

- high energy processing (e.g., spraying, grinding, hot processes) or low energy processing (e.g., assembly of article components, dipping of articles into vat);
- remote or intimate contact during normal operation; etc.

The ECHA R 12 Guidance: Use description proposes a standardised way of providing some of these information by using a battery of descriptors to define the use and the use conditions in a standardised way:

- LCS: Life Cycle Stages
- SU: Sector of Use
- PC: Product Category
- PROC: process category
- ERC: Environmental Release Category
- AC: Article Category
- TF: Technical Function

These descriptors are nowadays implemented in tools like ECETOC's TRA (Targeted Risk Assessment)[17]. for the exposure estimation and risk characterisation.

These descriptors are also implemented in the so called "Use maps" [18] developed by sector associations to provide information in a harmonised way on the manufacturing processes and operational conditions for the production of their products using these descriptors.

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[17] Available at: https://www.ecetoc.org/tools/tra-main/https://www.ecetoc.org/tools/tra-main/

[18] Available at https://echa.europa.eu/csr-es-roadmap/use-maps/concept

In Chesar these Use maps can be directly imported if they are available in the Chesar format. The sector use maps are helpful because they expedite the entry of input data into Chesar. But information about the processes and operational conditions can also be gathered in the supply chain. And inserted and modified manually in Chesar.

Based on these inputs and defining the conditions use, the corresponding exposure estimates are calculated and compared with the predicted no-effect concentrations for the environment (PNECs) and the derived no-effect levels for human health (DNELs)(ECHA, 2020).

For this case study, the plastic converter sector was identified as the sector that transforms (processes) plastics such as formulating the plastisol and producing plastic articles. Although the value chain of the plasticisers in the application of metal caps deviates from the traditional one and places other sectors and responsibilities in the value chain, it has been considered that activities in the processing of the plastics are similar. For this reason, the use maps developed by the European Plastic Converters Association (EuPC) (EuPC, 2016) have been used as a reference to build the exposure scenarios for the case study. However, these “Use maps” only contain the description of the processes and some general recommendation for the operational conditions. For this reason, these “Use maps” have been adapted to the case study afterwards as detailed information has become available.

2.3.2.3 Human health aspects

2.3.2.3.1 Hazard assessment

Hazard data and relevant physico-chemical properties were extracted from the respective REACH registration dossiers as published on the ECHA website. As such they were provided for import into the Chesar tool (v3.7.2)[19]. These data are summarized in Annex 3.

Only long-term systemic DNELs were considered relevant for worker risk assessment, as none of the substances are classified for local effects and since the exposure is either occupational or via diet, both of which are chronic exposure.

2.3.2.3.2 Exposure assessment

The sector-specific use map developed by the EuPC provided via the ECHA website[20], was imported into Chesar. The EuPC Use map covers the formulation of a plastisol (i.e., a plasticised PVC preparation) and the production of plastic articles (i.e., cap liners in this case study). Not every worker contributing scenario (CS) contained in the EuPC Use map is relevant for the production of cap liners. The CSs which only apply to plastic articles unrelated to FCM, were deleted from the life cycle tree.

The EuPC use map does not cover the manufacture of the plasticiser itself. Thus, a manufacture step with typical worker CSs for different manufacturing conditions was added to the overall life cycle in Chesar, preceding the formulation step.

The complete life cycle of the plasticiser used in cap liners and the associated CSs is shown in Table 15.

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[19] Available at: https://chesar.echa.europa.eu/-/chesar-3.7.2-available-for-download

[20] Available at: https://echa.europa.eu/documents/10162/2777483/eupc-eumbc_usemap_v1-0_en.chr3

Table 15. Plasticiser Life Cycle and Relevant Contributing Scenarios

MANUFACTURE		
Environment contributing scenario(s):		
CS 1	Manufacture of plasticiser	ERC 1
Worker contributing scenario(s):		
CS 2	SCC Production	PROC 1
CS 3	Continuous synthesis	PROC 2
CS 4	Batch synthesis	PROC 3
CS 5	Non-SCC Production	PROC 4
CS 6	Transfer, non-dedicated facility	PROC 8a
CS 7	Transfer, dedicated facility	PROC 8b
CS 8	Filling into small containers	PROC 9
CS 9	Quality control	PROC 15
FORMULATION		
Environment contributing scenario(s):		
CS 1	Production of a Plastisol	ERC 2
Worker contributing scenario(s):		
CS 2	Handling of Small Containers Containing Additive	PROC 9
CS 3	Handling Large Containers Containing Additive	PROC 8b
CS 4	Continuous Mixing Process	PROC 4
CS 5	Batch Mixing Process	PROC 5
CS 6	Laboratory/Quality Control Operations	PROC 15
ON-SITE USE		
Environment contributing scenario(s):		
CS 1	Production of Plastic Articles	ERC 5
Worker contributing scenario(s):		
CS 2	Handling of Small Containers Containing Masterbatches and/or Compounds	PROC 9
CS 3	Handling Large Containers Containing Masterbatches and/or Compounds	PROC 8b
CS 4	Handling of Small Containers Containing Additive	PROC 9
CS 5	Handling Large Containers Containing Additive	PROC 8b
CS 6	Use in a Closed and/or Semi-Open Converting Process (e.g. Extrusion, Injection)	PROC 14
CS 7	Use in an Open Converting Process (e.g. Calendering)	PROC 6
CS 8	Use in a Closed and/or Semi-Open Converting Process (Role and spread coating)	PROC 10
CS 9	Laboratory/Quality Control Operations	PROC 15
SERVICE LIFE		
Environment contributing scenario(s):		
CS 1	Use in gaskets for jars, bottles, etc. with food contact, outdoors	ERC 10a
CS 2	Use in gaskets for jars, bottles, etc. with food contact, indoors	ERC 11a
Consumer contributing scenario(s):		
CS 3	Consumption of food and drink in contact with cap liner	AC 13d

The end-of-life of the gasket is linked to the end-of-life of the cap which can be considered a single use packaging. There is no evidence that metal caps are actually recovered and recycled. Should that be the case and additional processing stage with its contributing scenarios should be assessed. For this case study, it is assumed that all the caps are part of the municipal waste flow.

Exposure assessments were conducted using the ECETOC TRA tool implemented in Chesar. In TRA, assessment of inhalation exposure to non-solid substances is driven by the vapour pressure (VP) of the substance and the PROC. TRA will group any substance into volatility ("fugacity") bands according to its VP (minimal / low / medium / high). All chemicals in this case study fall within the "minimal" fugacity band, but the cut-off for this band is as high as 500 Pa, which is 10000 times higher than the highest measured VP for any of the plasticisers in this case study. The TRA banding approach will therefore greatly overestimate the volatility of low-VP compounds. The VP typically represents ambient temperature (up to 40°C in TRA). For operations at higher temperatures, the assessor can enter a VP valid for this temperature. If no VP for the operation temperature is entered, TRA will assume the highest fugacity band, equivalent to a VP of >10000 Pa. Only DEHP had discrete VP values for the elevated temperatures available in its published registration dossier (60°C: 6E-7 Pa; 200°C: 39 Pa). These values were manually entered in Chesar. For all other substances, TRA used the default VP of 10000 Pa for processes at higher temperatures.

For each combination of PROC and fugacity band, TRA will assign an initial inhalation exposure estimate in the unit "ppm", which is then converted to mg/m^3 using the MW of the substance and the molar volume 24.45 L/mol. Hence, substances with higher MWs will have higher exposures in mg/m^3 units for the same prediction in ppm units. The initial inhalation exposure is reduced by RMMs such respiratory protection, local exhaust ventilation, or short exposure times. TRA predicts dermal exposures depending on the PROC. Again, the initial estimate can be reduced by external factors such as room ventilation or the wearing of protective gloves.

As not all the information with regards to the operational conditions (OCs) was available, for the purpose of the comparative assessment, identical OCs and risk-mitigation measures (RMMs) were used for all plasticisers and for each CS. For that aim basic RMMs that do not rely on personal protective equipment (PPE) which can be a burden if worn for an entire shift were chosen. For each CS an entire shift (≤ 8 h) was considered. Workers were considered to wear protective gloves with an effectiveness of ≥80%, but no respiratory protection. The room ventilation was considered "good," but only basic Local Exhaust Ventilation (LEV) with an effectiveness of 50-80% employed.

All assessed plasticisers are liquids, whereas the plastisol and the resulting cap liners are non-dusty solids. The mixing of plasticiser and PVC occurs at 60°C, whereas the production of the cap liners is conducted at temperatures of up to 200°C.

2.3.2.4 Other safety aspects

In this section other safety aspects related with the production and processing at the workplace are assessed.

2.3.2.4.1 Physico-chemical aspects

None of the plasticisers are classified for physical hazards that might raise safety concerns.

2.3.2.5 Environmental aspects

2.3.2.5.1 Environmental assessment

Hazard data and relevant physical-chemical properties were extracted from the respective REACH registration dossiers as published on the ECHA website. As such, they were imported into the Chesar tool (v3.7.2). These data are summarized in Annex 3.

The most important parameters to determine Predicted Exposure Concentration (PEC) values are:

- Ready biodegradability
- Water solubility
- Vapour pressure
- Partitioning coefficients organic matter in soil/water (Koc) or solvent/water (Kow).

The most important PNEC value is the value for surface water, because it allows to estimate the PEC values for sediment and soil (via the equilibrium partitioning method).

Certain amendments were made to the data if endpoints were missing but were regarded as critical for the environmental exposure and risk assessment. These additional values and explanatory comments are presented in Annex 4, Table A 7. For example, a vapour pressure of 0 Pa was reported for some of the substances, but 0 is not a value that allows the calculation of PEC values in the environment. Therefore, the value of 0 was replaced with a value near 0, i.e., 1.00E-09 has been inserted. Also, additional information on Henry Law constants was provided to JRC which was not included in the ECHA data sets. Furthermore, data gaps related to biodegradation and PNEC values for surface water were estimated based on QSAR.

As a result of the above-mentioned data gaps, the assessment would be partially based on experimental data and partially based on estimated data, hence, on data with variable robustness. For an alternative risk assessment, taking into account this possible bias, hazard data and relevant physical-chemical properties for all substances were generated based strictly on their molecular structure (simplified molecular-input line-entry system - SMILES codes) and the respective output of different QSAR tools. These data are summarized in Annex 3.

2.3.2.5.2 Exposure assessment

The sector-specific Use map developed by the association of European Plastics Converters (EuPC) provided via the ECHA website[21], was imported into Chesar. The EuPC use map covers the formulation of a plastisol (i.e., a plasticised PVC preparation; ERC2) and the production of plastic articles (i.e., cap liners in this case study; ERC5).

The EuPC Use map does not cover the manufacture of the plasticiser itself. Thus, a manufacture step with typical worker CSs for different manufacturing conditions and with ERC1 was added to the overall life cycle in Chesar, preceding the formulation step.

Exposure assessments were conducted using the European Union System for the Evaluation of Substances (EUSES)[22] 2.1.2 tool implemented in Chesar. EUSES 2.1.2 still applies SimpleTreat 3.1 and has been replaced by EUSES 2.2.0, but this is not considered to significantly impact the outcome of the present comparative assessment.

In order to focus on the comparative nature of the assessment, identical conditions of use and release settings were employed for all substances for each CS. Specifically, calculations were performed with a default annual volume of 1000 metric tonnes.

Environmental releases were assessed at the local and regional scale.

2.3.2.6 Results

2.3.2.6.1 Human health – Hazard assessment

DEHP is the only substance in this assessment that carries a classification according to the CLP criteria. DEHP is classified as a reproductive toxicant (Cat. 1B – H360). It causes testicular atrophy in rodents and foetotoxicity. The derived no-effect levels for human health (DNELs) for workers and the general population are based on the NOAEL of 4.8 mg/kg bw/day from a three-generation reproductive toxicity study. The critical effect in this study was testicular atrophy.

DEHA is not classified at all and no DNELs were available in the REACH Registration Dossier. Data from a report of the Danish Environmental Agency on Alternatives to classified phthalates in medical devices was used to fill these data gaps (DEPA, 2014).

Likewise, ATBC is of low toxicity and the long-term DNELs are derived from a No Observed Adverse Effect Levels for human health (NOAEL) of 100 mg/kg bw/day from one-year rat feeding study based on a body weight reduction in female rats.

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[21] Available at: https://echa.europa.eu/csr-es-roadmap/use-maps/concept

[22] Available at: https://echa.europa.eu/support/dossier-submission-tools/euses

The long-term DNELs for DINCH are derived from a NOAEL of 40 mg/kg bw/day found in a 2-year rat carcinogenicity study. The underlying critical effect is not disclosed in the published registration dossier.

For ESBO, only subacute toxicity data were available. The long-term DNELs were calculated using an extra assessment factor of 6 for extrapolation from subacute to chronic exposure. The NOEL of 1000 mg/kg bw/day from a combined repeated dose and reproduction / developmental screening study was used. No treatment-related adverse effects were seen.

The DNEL setting for DEHT is based on a 2-year feeding study in rats. A NOAEL of 79 mg/kg bw/day was used as point of departure. The underlying effects were limited to low weight gain and food conversion efficiency in male and female rats and ocular changes in female rats.

A summary of the DNEL values is presented in Table 16.

Table 16. Derived No-effect Levels for human health (DNEL) setting for workers

	DEHP	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Inhalation - long term DNEL (mg/m^3)	1.6	7.04	17.8	23.2	235	11.9
Point of departure	4.8 mg/kg/d, NOAEL, 3-gen study, oral, rat	100 mg/kg/d, NOEL, 2-year study, oral, rat	not reported	79 mg/kg/d, NOAEL, carcinogenicity, oral, rat	40 mg/kg/d, NOAEL, carcinogenicity, oral, rat	1000 mg/kg/d, NOAEL, 28-day study, oral, rat
Relative absorption	75 / 75 (oral/inhalation)	50 / 100 (oral/inhalation)	–	50 / 100 (oral/inhalation)	50 / 5 (oral/inhalation)	100 / 100 (oral/inhalation)
Overall assessment factor	7.5	12.5	–	3	3	600
Dermal - long term DNEL (mg/kg bw/day)	3.4	2	25.5	6.58	42	1.7
Point of departure	4.8 mg/kg/d, NOAEL, 3-gen study, oral, rat	100 mg/kg/d, NOEL, 2-year study, oral, rat	not reported	79 mg/kg/d, NOAEL, carcinogenicity, oral, rat	40 mg/kg/d, NOAEL, carcinogenicity, oral, rat	1000 mg/kg/d, NOAEL, 28-day study, oral, rat
Relative absorption	75 / 5 (oral/dermal)	100 / 100 (oral/dermal)	–	100 / 100 (oral/dermal)	50 / 4 (oral/dermal)	100 / 100 (oral/dermal)
Overall assessment factor	30	50	–	12	12	600

No investigated alternatives to DEHP are classified. The DNELs are based on unspecific high-dose effects like reduced body weight or liver weight increase. In contrast, DEHP is a classified reproductive toxicant and as such, a substance of very high concern (SVHC), as defined in the REACH regulation.

2.3.2.6.2 *Human health – Exposure Assessment*

Inhalation and dermal are the relevant exposure routes for workers. The exposure estimation and the Risk Characterization Ratios (RCRs) for the different contributions scenarios, are presented in Annex 6 and Figure 5, Figure 6 and Figure 7 illustrate these results for the manufacturing of the plasticisers, formulation of the plastisol and production of the gasket.

Figure 5. Risk Characterization Ratios (RCRs) for the manufacturing of the plasticisers

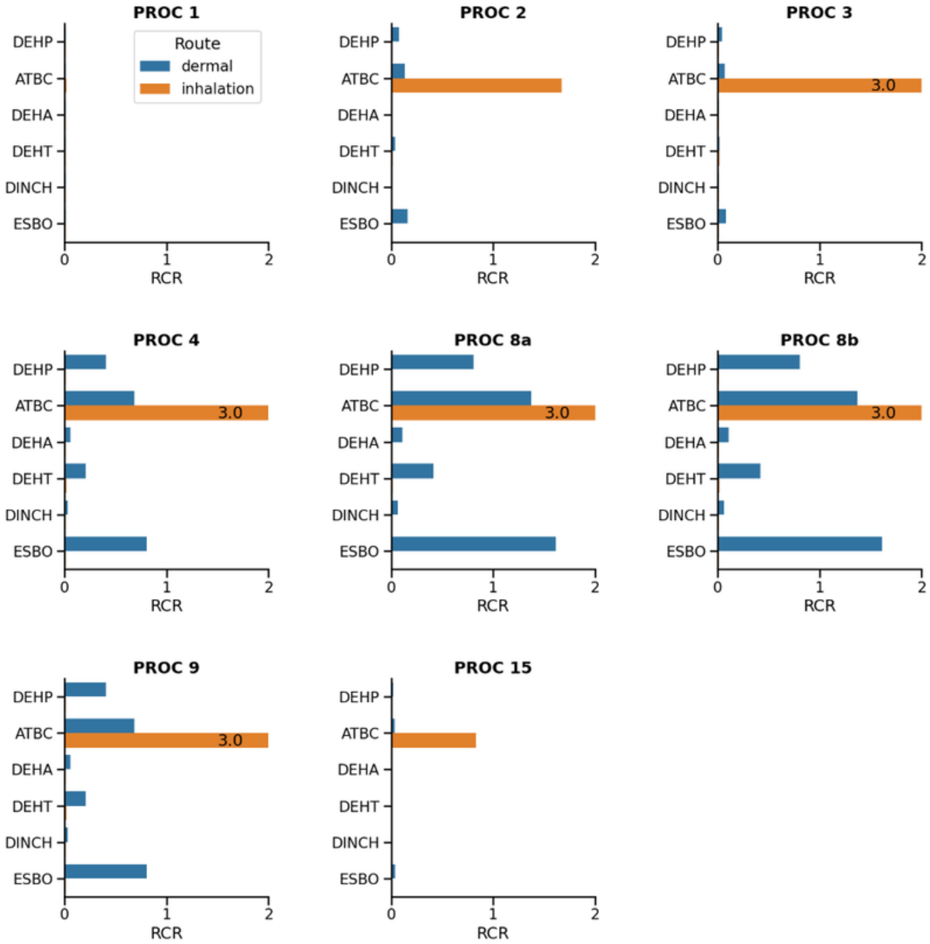


Figure 6. Risk Characterization Ratios (RCRs) for the formulation of the plastisol

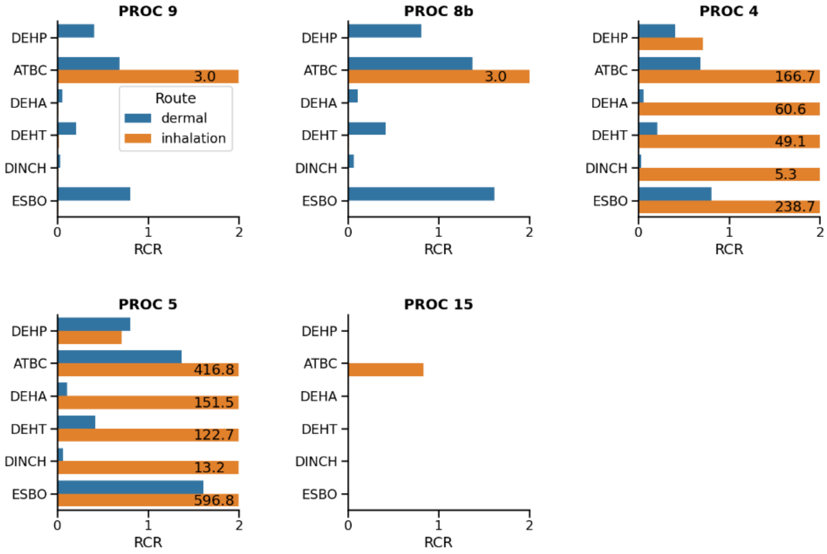
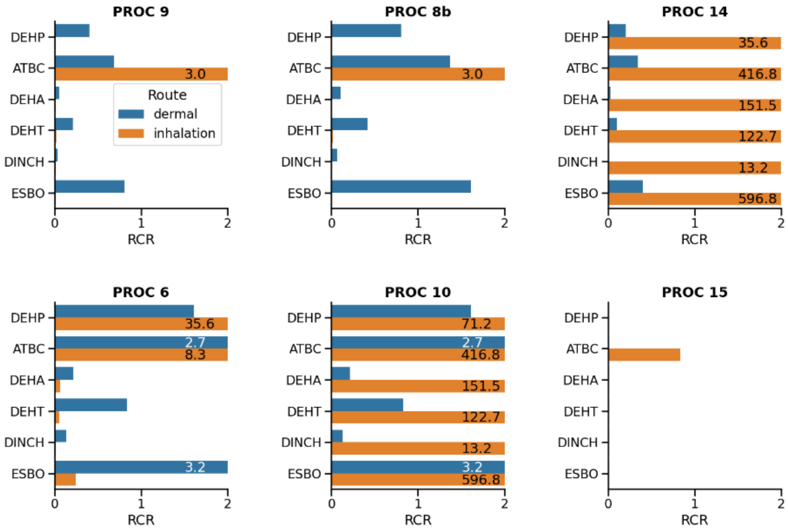


Figure 7. Risk Characterization Ratios (RCRs) for the production of the gasket



The relative risk for workers for the different substances strongly depends on the predicted air concentrations. Within the TRA model, inhalation exposure is determined by the vapour pressure of the substance and its concentration in the matrix being processed. If no vapour pressure is available for the given process temperature, TRA will group the substance into the highest volatility band.

ATBC has the highest vapour pressure, and the inhalation exposure estimates are higher than for the other plasticisers.

For DEHP, DEHT, and ESBO, vapour pressures of 0 Pa are reported for a temperature of 25 °C. Only the DEHP dataset contains distinct vapour pressures at elevated temperatures, so that TRA can use these values to predict the saturated vapour concentration (SVC) as worst-case exposure to the substance. If the vapour pressure at the process temperature is zero, the SVC and exposure will also be 0 mg/m^3. For all other substances, very high default concentrations are predicted for processes at temperatures higher than 40 °C, TRA's upper boundary for "ambient temperature".

On the other hand, DEHP has the lowest worker inhalation DNEL of all investigated substances, but it also has a low documented vapour pressure at temperatures of >200 °C. Therefore, TRA provides a more realistic estimate of inhalation exposure than for the other plasticisers.

The volatility of the investigated plasticisers is low. For substances with very low volatility, the precision and comparability of experimental vapour pressures is considered low. It may be more robust to use vapour pressures predicted by QSAR models than using experimental values with high uncertainty. On the other hand, one might also conclude that inhalation is not a relevant route of exposure for non-volatile plasticisers.

Dermal exposure estimates are identical for all substances in each CS. Thus, the Risk Characterization Ratios (RCRs) only depends on the magnitude of the dermal DNEL so that DINCH has the lowest dermal RCRs among all substances.

2.3.2.6.3 Environment - Hazard Assessment

Ecotoxicological data was available for the substances in the ECHA database, but was not complete. Since the Predicted No Effect Concentration (PNEC) for surface water is a key value, which allows the estimation of PNEC values for the marine environment as well as for sediment and soil via the equilibrium partitioning method, the PNEC surface water estimated for DEHP, DINCH and ESBO based on their SMILES code and using Ecosar. For ESBO, the PNEC STP (Sewage Treatment Plant) was also missing and was set to the same value as PNEC surface water.

For the marine compartments and predators, PNECs were not available for all substances but were not estimated.

A summary of the PNEC values is presented in Table 17.

Table 17. Predicted No Effect Concentration (PNEC) values of the plasticisers

	DEHP	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Freshwater (mg/L)	1.90E-05	2.20E-02	8.00E-05	8.00E-05	2.24E-06	2.10E-09
Sediment (freshwater) (mg/kg)	1.00E+02	4.15E+01	8.28E+00	8.28E+00	8.56E-01	1.00E+00
Marine water (mg/L)	No hazard identified	2.00E-03	No hazard identified	8.00E-06	No hazard identified	No hazard identified
Sediment (marine water) (mg/kg)	2.00E+01	4.15E+00	No hazard identified	8.28E-01	No hazard identified	No hazard identified
Sewage Treatment Plant (mg/L)	2.01E+02	1.00E+02	1.00E+00	1.00E+00	2.20E-06	1.00E-09
Air	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
Agricultural soil (mg/kg)	1.30E+01	8.29E+00	8.65E-01	1.50E-02	4.47E+01	6.25E+00
Predator’s prey (freshwater) (mg/kg food)	3.30E+00	1.05E+03	5.27E+01	5.27E+01	No potential	Insufficient data
Predator’s prey (marine water) (mg/kg food)	3.30E+00	1.05E+03	5.27E+01	5.27E+01	No potential	Insufficient data
Top predator’s prey (marine water) (mg/kg food)	3.30E+00	1.05E+03	5.27E+01	5.27E+01	No potential	Insufficient data
Predator’s prey (terrestrial) (mg/kg food)	3.30E+00	1.05E+03	5.27E+01	5.27E+01	No potential	Insufficient data

Rather low PNEC surface water values resulted from the assessment based on Smiles codes and they might be considered overly conservative. The values were nevertheless used because for compartments without PNEC values, Chesar does not estimate PECs and hence cannot assess any risks.

2.3.2.6.4 Environment – Exposure Assessment

Local and Regional Release before modelled Sewage Treatment Plant (STP)

Based on an annual production volume of 1000 metric tonnes, and according to the settings provided by the EuPC use map available on ECHA’s website, Chesar estimates the releases for all ERCs in Table 18. These releases are independent from substance specific parameters and are hence identical for all substances.

Even though the use map has been set up by the European industry, certain assumptions appear overly conservative. For example, the scenario ERC5 assumes 50% loss of the plasticiser to water (wastewater) and 50% to air. These values are consistent with the Organisation for Economic Co-operation and Development (OECD) guidance (ENV/JM/MONO(2004)8/REV1), but more realistic values can be concluded from the REACH guidance. Here, for Industry Category 11 (Polymer Industry), Use Category 47 (Softeners), EUSES would propose values from the REACH guidance, i.e., Table A 11, which describes emission factors to water between 0% and 0.1%, to air between 0.05% and 1% and to soil between 0.001% and 0.1% Table 18.

Table 18. Release information

Parameter	**ERC1**	**ERC2**	**ERC5**	**ERC11a**	**ERC10a**
Annual production volume (mt/year)	1.00 E+03	1.00 E+03	1.00 E+03	1.00 E+03	1.00 E+03
Annual total days	365	365	365	365	365
Annual production days	1.00 E+02	1.00 E+02	1.00 E+02	Not applicable	Not applicable
Annual use days	Not applicable	Not applicable	Not applicable	365	365

Parameter	ERC1	ERC2	ERC5	ERC11a	ERC10a
Daily production volume (mt/day)	1.00 E+01	1.00 E+01	1.00 E+01	2.74E+00	2.74E+00
Release factor water	6.00 E-02	2.00 E-02	5.00 E-01	5.00 E-04	3.20 E-02
Release factor air	5.00 E-02	2.50 E-02	5.00 E-01	5.00 E-04	5.00 E-04
Release factor soil	1.00E-04	1.00E-04	1.00E-02	0	3.20 E-02
Release rate local water (kg/day)	6.00E+02	2.00E+02	5.00E+03	2.74E-04	1.75E-02
Release rate local air (kg/day)	5.00E+02	2.50E+02	5.00E+03	2.74E-04	2.74E-04
Release rate local soil (kg/day)	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.75E-02
Release rate regional water (kg/day)	1.64E+02	5.48E+01	1.37E+03	1.37E-01	8.77E+00
Release rate regional air (kg/day)	1.37E+02	6.85E+01	1.37E+03	1.37E-01	1.37E-01
Release rate regional soil (kg/day)	2.74E-01	2.74E-01	2.74E+01	0	8.77E+00

Distribution in the modelled *Sewage Treatment Plant (*STP)

Generally local releases to water are considered to happen through the releases to the wastewater and to undergo a substance-specific distribution in the STP. The key properties that determine this distribution are biodegradability, Kow, vapour pressure and molecular weight. Henry constant (HLC) and Koc can then be calculated or estimated if no measured data is available. These key parameters are summarized in Table 19.

Table 19. Properties to determine distribution

	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Molecular weight in g/mol	390.56	402.5	370	390.6	424.6	974.71
Vapor Pressure in Pa at 25°C	1.00E-09 *	4.90E-02	1.00E-09 *	1.00E-03	2.20E-05	1.00E-09 *
HLC in Pa m^3/mol at 25°	1.30E-02	4.43E+00	4.40E-02	1.034E+04	7.16	4.55E-02 **
Log Kow	7.5	4.86	8.94	5.2	10	6.2
Koc	1.50E+06	1.87E+04	3.63E+04	2.69E+05	3.89E+06	1.00E+10
Biodegradation	readily biodegradable	Inherently biodegradable	readily biodegradable	readily biodegradable	not readily biodegradable ***	readily biodegradable

*Estimated because calculations cannot be performed with vapour pressure = 0 Pa m^3/mol

**Estimated based on vapour pressure and water solubility

***In the alternative QSAR based calculation, it is assumed that DINCH is inherently biodegradable. This will, however, not change the distribution in the STP according to the model.

The distribution fractions of the substances in the STP for the compartments air, water, sludge and biodegradation were calculated by Chesar with SimpleTreat[23] Table 20.

Table 20. SimpleTreat 3.1 results

	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
FSTP,air	4.85E-07	1.11E+00	6.75E-06	1.70E-02	1.20E-02	2.93E-08
FSTP,water	7.77E+00	3.31E+01	6.79E+00	7.12E+00	8.17E+00	8.00E+00
FSTP,sludge	8.96E+01	6.58E+01	6.17E+01	8.19E+01	9.18E+01	9.20E+01
Biodegradation	2.67E+00	0.00E+00	3.15E+01	1.10E+01	0.00E+00	4.36E-04
Total	1.00E+02	1.00E+02	1.00E+02	1.00E+02	1.00E+02	1.00E+02

FSTP = distribution fractions of the substances in the Sewage Treatment Plant

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[23] SimpleTreat is an exposure and emission model developed to estimate chemical emission from sewage treatment plants and exposure in surface water within the framework of risk assessment of chemicals.

The values indicate that despite ready or at least inherent biodegradability, DEHP, DEHA, ATBC, ESBO and also DEHT do not show any or no significant degradation in the STP.

According to the SimpleTreat model, due to high Kow or Koc values of substances, sorption to sludge takes place before significant biodegradation occurs. Consequently, the sludge as well as the effluent water contain high concentrations of the substances. This might be an overly conservative approach and more robust and accurate results could be obtained from higher tier degradation studies with these substances.

Releases from the modelled Sewage Treatment Plant (STP)

For the scenarios ERC1, ERC2 and ERC5, local PEC values result predominantly from the local releases to wastewater and from the STP via the effluent to surface water and sediment and via the sludge to agricultural soil. For the scenarios ERC11a and ERC10a, since the local releases to wastewater are much lower than in the other scenarios, the local PEC values are relatively seen more impacted by regional releases and distribution processes.

Distribution in other environmental compartments

Also, the direct releases to air, followed by deposition to surface waters and soil, are simulated based on various partitioning coefficients, that are mainly determined by the same parameters mentioned above, i.e., Kow, Koc, vapour pressure, HLC, water solubility and degradation characteristics. All these parameters vary between the substances and result in different distribution patterns. These regional and continental distribution processes were not analysed in detail as part of this study.

2.3.2.7 Discussion

2.3.2.7.1 Human health

The relative risk for workers for the different substances strongly depends on the predicted air concentrations. ECETOC TRA can limit inhalation exposure to the saturated vapour concentration (SVC) of the substance, but this only works if a defined value for the vapour pressure at the selected process temperature is entered into ECETOC TRA. This is the reason why DEHP has a lower inhalation RCR than some alternative plasticisers, despite their higher inhalation DNELs. For substances with very low volatility, the precision and comparability of experimental vapour pressures is considered low. It may be more robust to use vapour pressures predicted by QSAR models than using experimental values with high uncertainty. An exemplary exposure estimation using only QSAR-predicted vapour pressures (Modified Grain Method, Annex 3) has been conducted for the handling of the plastisol formulation prior to the production of the cap gaskets (PROC 8b, Figure 8) , which is a process at ambient temperature. The available QSAR methods cannot predict the vapour pressure at elevated temperatures. For the hot processes, TRA will use generic conservative vapour pressure estimates, which are identical for all plasticisers studied here (i.e., 1E+4 Pa at 200°C), unless a defined vapour pressure for the process temperature is used to override the default estimate (these are available only from the vapour pressure study DEHP).

On the other hand, one might altogether conclude that inhalation is not a relevant route of exposure for non-volatile plasticisers.

For dermal exposure, all exposure predictions by TRA are identical, regardless of the substance. The concentration of the plasticiser in the process is not accounted for. In this case study, this is not important since all plasticisers are employed at a similar concentration of 31-35%.

Dermal absorption information is not available for the plasticisers in question. If this were available, it should have been used to refine the dermal DNELs. In any case, dermal absorption is expected to be very low due to the relatively high molecular weight and the very high lipophilicity of the plasticisers.

The plasticisers in this case study have a high molecular weight (ca. 400 g/mol, up to >900 g/mol). And log Kow values are very high (≥5). Both factors contribute to a very low predicted dermal penetration. For DEHP, a dermal absorption of only 0.64% was measured in rats. Molecules with similar properties (Molecular Weight (MW), Log Kow, water solubility) will show similarly low dermal penetration. What comes into contact with the skin will not be absorbed to an appreciable extent. Thus, they are likely to adhere to the outmost layers of the skin and not penetrate into viable skin layers where systemic uptake can occur. Therefore, dermal contact, like inhalation, may be considered an unlikely route for systemic exposure to plasticisers. But ECETOC TRA does not deal with systemic exposure, only external exposure, and this could lead to an overestimation of health risks via dermal route.

Another factor is the DNEL setting. DNELs are set by the registrants based on heterogeneous databases with sometimes not completely transparent choices of assessment factors. Different registrants have followed different approaches for setting DNELs. Furthermore, the severity of an effect defining the NOAEL / DNEL can differ substantially. DNELs for ATBC and ESBO used NOELs based on from marginal, adaptive effects like liver weight increase as point of departure, i.e., the NOAEL for truly adverse effects could be much higher, but the DNEL does not reflect this.

Taken together the different approaches for DNEL setting and the different effects underlying the point of departure, the magnitude of the DNEL is not necessarily a good measure for the toxicity of a substance.

Whereas improving the quality of the DNELs is outside the scope of this project, for those exposure Scenarios for which the exposure estimates exceed the DNELs, additional measures to mitigate the risk need can be considered. Measures like the duration of the activity, the Local Exhaust Ventilation and as last resource Personal Protective Equipment.

Based on feedback received from the sector industry additional measures like the use of FFP2 face masks with a respiratory protection of Assigned Protection Factor >10 and Chemical resistant gloves (tested to EN374) in combination with 'basic' employee training (effectiveness >%95) have been applied.

After applying these additional measures, as it can be seen in Figure 8, Figure 9. and Figure 10 the exposure and therefore the risk is reduced compared with Figure 5, Figure 6 and Figure 7 in all the process making the RCR be lower than 1 in most of the cases.

Figure 8. Reviewed Risk Characterization Ratios (RCRs) plasticiser production

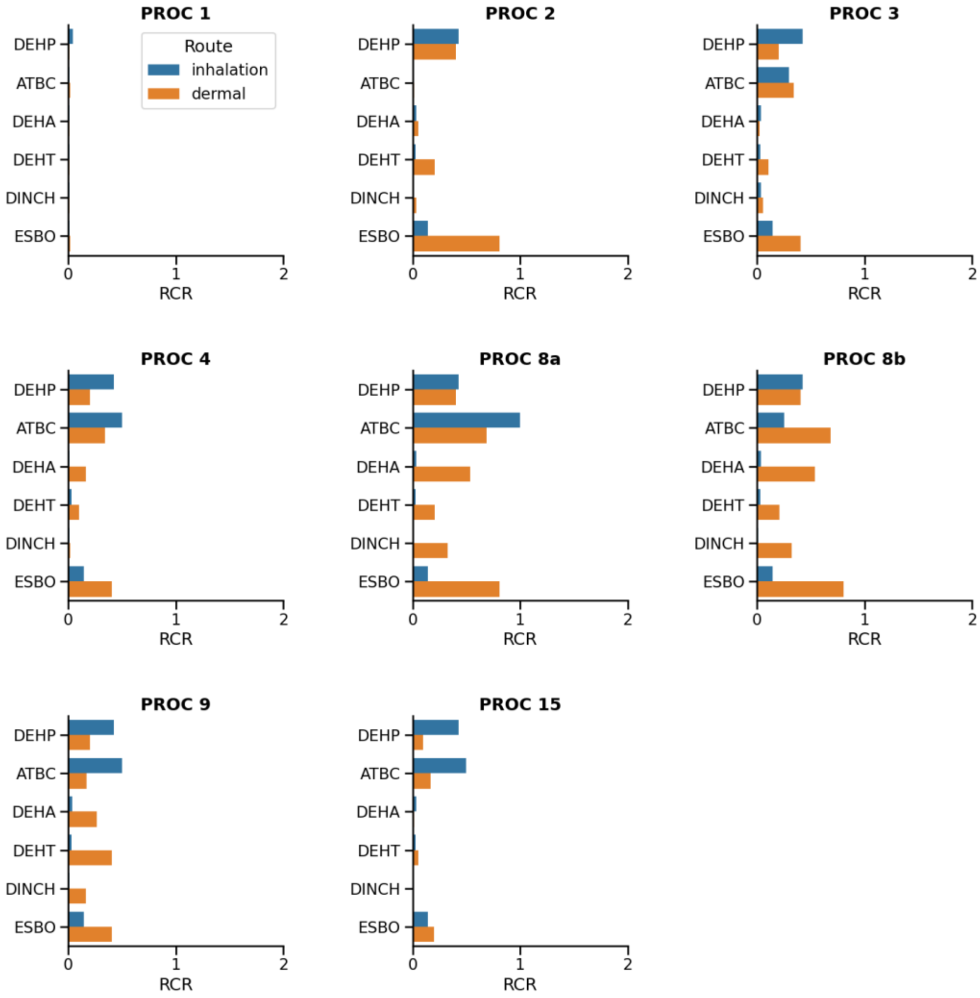


Figure 9. Reviewed Risk Characterization Ratios (RCRs) plastisol formulation

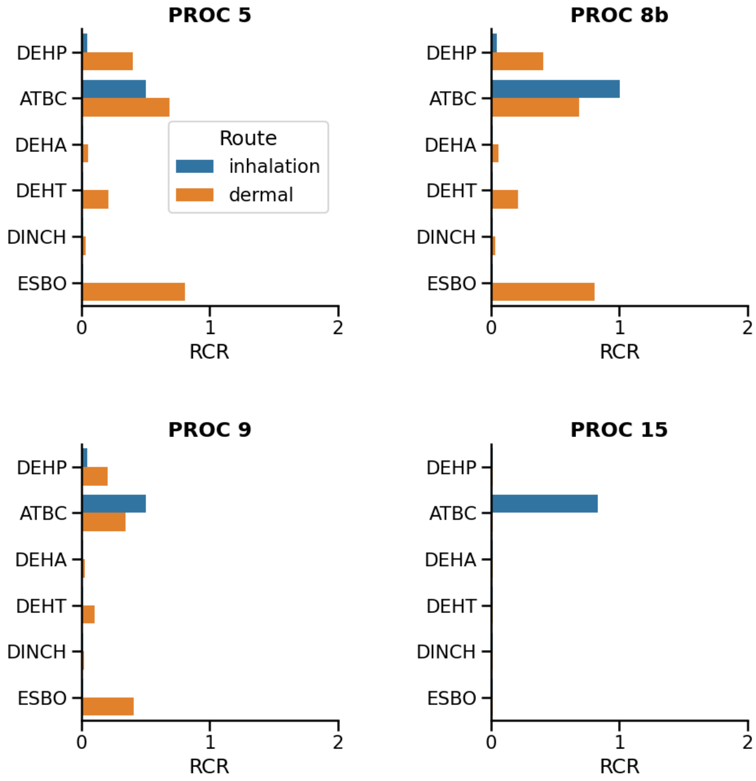
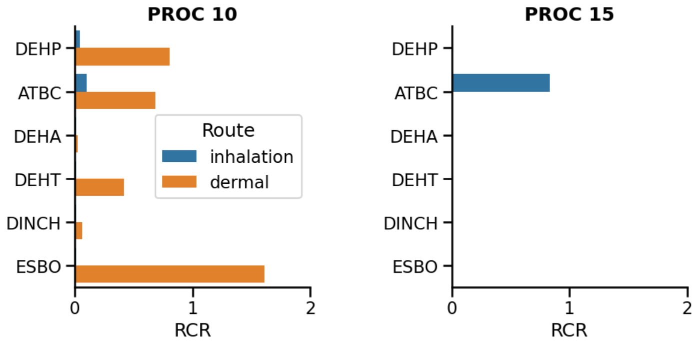


Figure 10. Reviewed Risk Characterization Ratios (RCRs) gasket production



The details of the exposure estimation values and the RCRs after applying these additional measures are presented in Annex 5.

2.3.2.7.2 Environment

Comparative Ecotoxicological Profiles

A selection of key PNECs has been summarized in Table 21 to illustrate whether a consistent hazard profile can be assigned to the substances. It can be concluded though that the level of aquatic and terrestrial toxicity varies. For example, DINCH has the lowest PNEC for aquatic organisms and at the same time the highest PNEC for terrestrial organisms.

Table 21. Predicted No Effect Concentrations (PNECs) values

PNECs	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Fresh water (mg/L)	1.90E-05	2.20E-02	8.00E-05	8.00E-05	2.24E-06	2.10E-09
Sediment (freshwater) (mg/kg dw)	1.00E+02	4.15E+01	8.28E+00	8.28E+00	8.56E-01	1.00E+00
Agricultural soil (mg/kg dw)	1.30E+01	8.29E+00	8.65E-01	1.50E+01	4.47E+01	6.25E+00

The alternative PNECs, estimated based on the molecular structure and on QSAR endpoints only, result in a more consistent picture, as presented in the Table 22.

Table 22. QSAR Estimated Predicted No Effect Concentrations (PNECs) values

PNECs	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Fresh water (mg/L)	1.90E-05	1.16E-02	2.77E-05	1.90E-05	2.24E-06	2.10E-09
Sediment (freshwater) (mg/kg dw)	6.36E-05	1.74E+00	9.28E-05	6.36E-05	7.50E-06	7.03E-09
Agricultural soil (mg/kg dw)	4.14E-06	3.38E-01	5.05E-06	8.09E-06	1.14E-06	3.49E-10

For a comparative environmental risk assessment of different substances, it is important to verify that the PNECs were set based on equally robust data. If the PNECs for one substance were derived using QSAR tools or were based only on acute aquatic toxicity data with a high assessment factor, while for another substance higher tier ecotoxicological data was available and PNECs were set based on a low assessment factor, this can lead to biased conclusions. For example, the PNECwater of ESBO was derived from Ecosar based on the Smiles code and is extremely low. If the PNECsediment and the PNECsoil are derived via Partitioning Equilibrium, they are much lower than actually measured values.

Comparative Environmental Fate Profiles

For the selected environmental compartments surface water, sediment and soil, the PEC values calculated by Chesar were compared to understand whether a consistent distribution profile can be assigned to the substances (see Table 23).

Table 23. Calculated Predicted Environmental Concentrations (PECs)

Regional PECs	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Fresh water (mg/L)	2.62E-04	2.74E-03	1.48E-03	4.64E-04	1.81E-04	2.41E-07
Sediment (freshwater) (mg/kg dw)	7.18E+01	9.83E+00	1.05E+01	2.49E+01	1.41E+02	4.82E+02
Agricultural soil (mg/kg dw)	5.60E-02	9.02E-03	5.50E-02	7.00E-02	2.72E-01	7.80E+01

There is a certain consistency in that ATBC and ESBO result in the highest and lowest PEC values. However, as expected, an inverse situation can be described between the compartment water on the one hand and the compartments sediment/soil on the other hand. The compartments are in a competitive situation for the substances due to sorption processes. For example, ATBC has the highest regional PEC in freshwater and at the same time the lowest PECs in sediment and soil, while ESBO has lowest regional PEC in freshwater and the highest PECs in sediment and soil.

The alternative PECs, estimated based on QSAR endpoints, result in somewhat different values but in a similar pattern, as presented in Table 24.

Table 24. Calculated Predicted Environmental Concentrations (PECs) using QSAR endpoints

Regional PECs	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Fresh water (mg/L)	1.70E-03	4.84E-04	5.03E-04	5.25E-04	3.05E-04	1.11E-05
Sediment (freshwater) (mg/kg dw)	2.58E-01	1.85E+01	9.86E+00	2.31E+01	1.02E+02	6.36E+02
Agricultural soil (mg/kg dw)	1.32E-03	1.37E-01	8.89E-03	7.24E-03	2.27E+00	7.69E+01

Comparative Environmental Risk Profiles

Finally, for the selected compartments also the respective RCRs are compared in Table 25. The level of the actual RCRs and the fact, whether risks are controlled or not, were not subject to the assessment. A detailed discussion on the conservative nature of the present assessment is provided in chapter 2.2.2.9.2. Despite the differences in the environmental hazard profiles and in the environmental fate profiles, now a consistent risk profile can be seen. Clearly, ATBC, even though no conclusion is yet available on its PBT status, shows the lowest RCRs (most favourable) in the selected compartments, both aquatic and terrestrial, and ESBO shows the highest RCSs (least favourable) in these compartments.

Table 25. Regional Risk Characterization Ratios (RCRs)

Regional RCRs	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Fresh water	1.38E+01	1.25E-01	1.85E+01	5.80E+00	8.08E+01	1.15E+02
Sediment (freshwater)	7.18E-01	2.37E-01	1.27E+00	3.00E+00	1.65E+02	4.82E+02
Agricultural soil	4.31E-03	1.09E-03	6.36E-02	4.67E-03	6.09E-03	1.25E+01

The alternative RCRs, estimated based on QSAR endpoints, result in different values but in a similar pattern, as presented in Table 26.

Table 26. Regional Risk Characterization Ratios (RCRs) using QSAR endpoints

Regional RCRs	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Fresh water	2.65E+01	1.47E-01	1.75E+01	2.76E+01	1.36E+02	5.29E+03
Sediment (freshwater)	1.55E+05	1.48E-01	1.99E+05	3.63E+05	1.37E+07	9.05E+10
Agricultural soil	2.15E+03	3.91E-03	2.71E+04	8.95E+02	1.99E+06	2.20E+11

Other Compartments and non-target Species

Chesar only partially estimated PEC values and RCR values for the marine compartments and for predators. Since information was not available for all substances, this comparative assessment addresses mainly the available information on surface water, sediment and soil.

2.3.2.8 SSbD Step 2 Scoring system

Different Contributing Scenarios/process (CS) operations contribute to overall assessment of the production, processing stages. In these contributing scenarios, exposure might happen via different routes. But not all of them are applicable in all cases. Taken this into consideration, an option for possible scoring for each contributing scenario could be as presented in Table 27. Each CS will be defined by a process categories (PROC) or an environmental release concentrations (ERCs).

Table 27. Options for possible scoring

For each CS: PROC and ERC	
If total RCR<1	3
If total RCR>1 but all individual RCRs<1	2
If total RCR>1 but at least 1 individual RCRs>1	1
If total RCR>1 and more than one individual RCRs>1	0

Each stage (manufacturing of the plasticiser, formulation of the plastisol and production of the gasket) will have a number of CSs PROCS and ERCs) scored 0-3. Table 28, Table 29 and Table 30 present the scores obtained for the manufacture of the plasticisers, formulation of plastisol, and the production of gaskets.

Table 28. Score for the different PROCs for human Health and ERC for Environment in the manufacturing of plasticisers

	Human Health								**Environment**
CSs	**PROC 1**	**PROC 2**	**PROC 3**	**PROC 4**	**PROC 8a**	**PROC 8b**	**PROC 9**	**PROC 15**	**ERC1**
DEHP	3	3	3	3	3	3	3	3	0
ATBC	3	3	3	3	1	3	3	3	0
DEHA	3	3	3	3	3	3	3	3	0
DEHT	3	3	3	3	3	3	3	3	0
DINCH	3	3	3	3	3	3	3	3	0
ESBO	3	3	3	3	3	3	3	3	0

Table 29. Score for the different PROCs for human Health and ERC for Environment in the formulation of plastisol

	Human Health					**Environment**
CSs	**PROC 5**	**PROC 8a**	**PROC 8b**	**PROC9**	**PROC15**	**ERC2**
DEHP	3	3	3	3	3	0
ATBC	1	2	1	3	3	0
DEHA	3	3	3	3	3	0
DEHT	3	3	3	3	3	0
DINCH	3	3	3	3	3	0
ESBO	3	3	3	3	3	0

Table 30. Score for the different PROCs for human Health and ERC for Environment in the production of gaskets

	Human health				**Environment**
	PROC5	**PROC8a**	**PROC8b**	**PROC10**	**ERC5**
DEHP	3	3	3	3	0
ATBC	1	2	1	3	0
DEHA	3	3	3	3	0
DEHT	3	3	3	3	0
DINCH	3	3	3	3	0
ESBO	3	3	3	1	0

2.3.2.9 Conclusions for step 2

2.3.2.9.1 Human health

The risk assessment of workers during production and use of plasticisers is hampered by uncertainties regarding volatility, dermal uptake, and the quantitative hazard assessment. However, due to the very low volatility and the expected very low potential for dermal uptake, the overall systemic exposure and risk for workers is considered low.

In addition to the uncertainties regarding plasticisers' properties, the exposure scenarios have been built based on very conservative working condition considerations due to the lack of specific information. It has been demonstrated, however, that little changes in these operational conditions provide significant changes in the characterisation of the risk. It is, therefore, necessary that all the possible data is available in order to be able to perform a more realistic assessment.

2.3.2.9.2 Environment

In order to support a reliable comparative environmental risk assessment of substances, hazard and environmental fate data for the respective substances should be equally robust. If higher tier studies are available for some substances, while only QSAR estimates are available for others, a biased outcome is likely.

Using QSAR models to predict these endpoints could be an alternative to ensure consistency of data especially for comparative assessment purposes. However, the applicability domain of some QSAR models can limit this possibility.

Likewise, for such substances, especially if the substances have low water solubility and high sorption affinity, also experimental data needs to be carefully assessed. Certain substance properties bring along analytical and methodological constraints and require expert knowledge during study conduct and study interpretation.

However, when robust environmental data is available and when this data has been assessed under REACH following similar guidance and scrutiny, the tool Chesar can be considered to allow a reliable comparative assessment for each environmental compartment. The present assessment also shows that QSAR modelling can be a reliable alternative.

Principally, comparative environmental assessments could lead to the conclusion that a single substance does not have the lowest risk for all compartments at the same time. In such case, a careful evaluation of the protection goals and of feasible risk mitigation measures should follow. In the case that was subject to this specific analysis as part of the SSbD, a recommendation could be made to focus further on the substance ATBC. As shown in Table 24 and Table 26, ATBC appears to have a more beneficial environmental profile than the low-molecular phthalate, di-2-ethylhexyl phthalate (DEHP). The substance ESBO instead, came out with the most unfavourable environmental profile. Whether this may be due to limitations of QSAR modelling and/or experimental approaches would need to be further investigated. Moreover, and as it happens for the human health assessment, the exposure scenarios have been built based on very conservative EUSES default values, that due to the lack of information have been used for the exposure estimations.

These default release fractions to water are in the range of 0.02 to 0.50 and may not reflect the current standard of manufacturing, formulation and production activities in Europe. To meet environmental standards (e.g. those set by the water framework legislation) it is necessary to implement process controls such as on-site wastewater treatment, waste gas treatment, waste incineration etc.

In fact, a publicly available extended Safety Data Sheet (e-SDS) for DEHP[24], shows that the majority of releases during the production and further processing of the plasticisers are effectively avoided by the risk mitigation measures in place. Realistic values for release fractions to water are described to be in the range of 3E-11 up to 5E-05. This means that default values are too high by a factor in the range of 2E+04 to 1E+09. Releases to soil can even be set to zero according to the extended Safety Data Sheet.

Therefore, applying more realistic release factors would improve the risk assessment significantly both at the local and regional level and providing an overall SSbD scoring as illustrated in Table 31.

Table 31. Overall SSbD scoring for the 6 plasticisers after the refinement for Environmental assessment

	Manufacture		**Formulation**		**Plastic article**	
	HH	**ENV**	**HH**	**ENV**	**HH**	**ENV**
DEHP	3	3	3	3	3	3
ATBC	3	3	2	3	2	3
DEHA	3	3	3	3	3	3
DEHT	3	3	3	3	3	3
DINCH	3	3	3	3	3	3
ESBO	3	3	3	3	3	3

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[24] Accessible at: http://www.oltchim.ro/en/uploaded/2011/SDS/DOP_eSDS_rev0_eng.pdf

2.3.3 Step 3 Human health and environmental aspects in the final application

2.3.3.1 Goal and scope

The goal of this step is to identify if the use of the product, in this case the gasket, in which the chemical/material the plasticiser, has been incorporated poses any risk for the consumer and the environment in relation to that chemical/material.

2.3.3.2 Approach

The approach to assess the human health and environmental safety in this case study differs from the usual risk assessment. In this case the exposure of the human health to the plasticisers is considered an indirect or secondary exposure because the human is exposed by ingestion to the plasticisers through the food.

The safety aspects of this application and the data requirements fall under the scope of Regulation 10/2011 (EC, 2011) on plastic materials and articles intended to come into contact with food.

Whether or not a health risk exists due to the intake of a substance with a certain hazard potential depends on the quantity ingested (exposure) and the exposure has to be below the Tolerable Daily Intake (TDI).

The TDI is an estimate of the amount of a chemical in air, food or drinking water that can be taken in daily over a lifetime without appreciable health risk. TDIs are calculated on the basis of laboratory toxicity data to which uncertainty factors are applied. The TDIs[25] for the plasticisers of the case study are reported in Table 32.

Another important parameter used as reference to determine whether a risk is controlled is the Specific Migration Limit of the chemical (SML) derived from the TDI values (EC, 2011). For the plasticisers with no Specific Migration Limit, the group Migration Limit (SML(T)) of 60 mg/Kg has been assigned.

A third parameter that could be used to compare with the exposure estimation is the DNEL for oral route.

Table 32. Tolerable Daily Intake for the Plasticisers

	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
TDI (mg/kg bw/day)	0.05	1	0.3	1	1	1
SML (mg/kg)	1.5	60	18	60	60	60
DNEL (mg/kg bw/day)	0.036	1	1.3	3.95	2	0.8

Regulation 10/2011 requires compliance testing to ensure that the migration of the plastic food contact materials do not exceed the limits set by the law.

For the exposure estimation, as an alternative to experimental testing, estimation of specific migration is permitted using generally recognised models as a good manufacturing practice, quality assurance, and compliance tool (Plastics Europe, 2021).

Migration is a global term to describe a net mass transfer of chemical substances from a packaging material into the food (Crompton, 2007). In the case of plastic food contact materials (FCM) covered by Regulation (EU) No 10/2011, migration includes several macroscopic mass transfer mechanisms including: i) mass diffusion in and through the different plastic materials as well as the liquid or gas phases separating the primary source from the food, and ii) desorption/sorption at the interface between each crossed medium (Brandsch et al., 2015).

For the purpose of illustrating how the results of the assessment can vary depending on the data/information availability, three different approaches/tools and scenarios have been used. The tools are presented from the most conservative to the most realistic one, based on the data requirements to simulate/estimate the migration and the consequent exposure. However, these approaches do not simulate the real scenario, as normally food is not in contact with the plasticised material in a jar.

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[25] Retrieved from https://www.efsa.europa.eu/it/data-report/chemical-hazards-database-openfoodtox

As regards to the environmental safety, how the activities in Step 2 and Step 3 contribute to the overall releases and risks has been assessed.

2.3.3.3 Chesar

2.3.3.3.1 Methodology

To assess the consumer safety aspects related to plasticisers in the cap liners, the article category AC 13d (Plastic articles intended for food contact) and the Environmental Release Categories ERC 10a 11a (Widespread use of articles with high or intended release (outdoor) and ERC 11a (Widespread use of articles with low release (indoor) were added as service life stage to the life cycle.

The service life CSs are shown in Table 33.

Table 33. Service life contributing scenarios (CS)

Service life		
Environment contributing scenario(s):		
CS 1	Use in gaskets for jars, bottles, etc. with food contact, indoors	ERC 11a
CS 2	Use in gaskets for jars, bottles, etc. with food contact, outdoors	ERC 10a
Consumer contributing scenario(s):		
CS 2	Consumption of food and drink in contact with cap liner	AC 13d

Human health exposure assessments were conducted using the TRA tool implemented in Chesar with identical use conditions for all plasticisers. Environmental Exposure assessments were conducted using the EUSES tool implemented in Chesar.

To assess exposure of consumers to plasticisers migrated into food, published migration data was used. For each substance, the worst-case measured concentration in food was adopted for the relevant TRA Consumer model in Chesar (Table 34). The model was set to “Child” as the most vulnerable subpopulation, with a default body weight of 10 kg. The volume of consumed food swallowed was arbitrarily set to 100 mL per day.

Table 34. Worst-case measured concentrations in food

	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Migration into food (% in food)	4.3E-2	2.2 E-2	1.1 E-2	6.6 E-4	2.5 E-3	6.5 E-2
Food	mussels in oil	mussels in oil	garlic in oil	garlic in oil	sesame paste	olive paste
Reference	Fankhauser-Noti Grob, 2006	Fankhauser-Noti Grob, 2006	Fankhauser-Noti Grob, 2006	Biedermann et al., 2022	Biedermann et al., 2022	Fankhauser-Noti Grob, 2006

For the environmental exposure assessment, a company produces a volume of 1000 metric tonnes per year is assumed. Estimated of the releases for the relevant ERCs is presented in Table 35. These releases are independent from substance specific parameters and are hence identical for all substances.

Table 35. Estimated releases for ERC11a and ERC10a

Parameter	**ERC11a**	**ERC10a**
Annual production volume (mt/day)	1000	1000
Annual total days	365	365
Daily production volume (mt/day)	2.74E+00	2.74E+00

Parameter	**ERC11a**	**ERC10a**
Release factor water	5.00E-04	3.20E-02
Release factor air	5.00E-04	5.00E-04
Release factor soil	0	3.20E-02
Release rate local water (kg/day)	2.74E-04	1.75E-02
Release rate local air (kg/day)	2.74E-04	2.74E-04
Release rate local soil (kg/day)	0.00E+00	1.75E-02
Release rate regional water (kg/day)	1.37E-01	8.77E+00
Release rate regional air (kg/day)	1.37E-01	1.37E-01
Release rate regional soil (kg/day)	0.00E+00	8.77E+00

Local releases are linear to the release rates and are therefore highest for Step 2 scenarios (ERC1, ERC2 and ERC5) and lowest for the Step 3 scenarios ERC11a and EWC10a. Instead, regional exposures are aggregated across all contributing scenarios and Chesar does not provide the contribution of each individual scenario to regional PEC values. In order to assess the respective contributions of Step 2 and Step 3 to the environment, the following calculations were performed and compared:

- For the contribution of Step 2 activities: The volumes of the Step 3 activities in the Use Map were set to zero. This allowed the determination of Step 2 contributions only.
- For the contribution of Step 3: The volumes of the Step 2 activities were set to zero. This allowed the determination of Step 3 contributions only.

2.3.3.3.2 Results and discussion

The ECETOC TRA consumer model for oral uptake simply multiplies the amount of food or drink consumed with the frequency of consumption and the concentration of the substance in food, divided by a default body weight for the subpopulation in question.

There is no migration data generated under identical, controlled conditions for all investigated plasticisers. Since all plasticisers are highly lipophilic with log Kow values ranging from 4.9 to 10, it is not surprising that researchers specifically analysed oil-based food for plasticiser migration from cap gaskets. The published results are used for this exposure assessment. The exposure estimated can be found in Table 36.

Table 36. Exposure estimation and Risk Characterization Ratios (RCRs) values for the consumption of food in contact with the cap liner

Route of exposure and type of effects		Oral exposure (mg/kg bw/day) / RCR = Exposure ÷ DNEL
DEHP	**Exposure**	4.3
	RCR	**119.4**
ATBC	**Exposure**	2.25
	RCR	**2.25**
DEHA	**Exposure**	1.15
	RCR	**0.885**
DEHP	**Exposure**	4.3
	RCR	**119.4**
DEHT	**Exposure**	0.066
	RCR	**0.017**
DINCH	**Exposure**	0.25
	RCR	**0.125**
ESBO	**Exposure**	19.5
	RCR	**24.37**

Since the plasticiser concentrations in food are measured values, consumer exposure predictions are considered a good estimation of the real-life exposure to these substances in food. However, a comparative migration experiment using an oily food simulant under controlled conditions would be the best option for assessing the relative exposure to plasticisers from cap gaskets.

Regarding the hazard part of the risk assessment, the same considerations regarding DNEL setting apply as for the worker DNELs: the magnitude of the consumer DNEL depends on the point of departure and the choice of assessment factor. The severity of the critical effect is normally not reflected in the DNEL.

As regards the environment, nearly 100% of all regional PEC values result from Step 2. The results are presented in Table 37 for the compartments surface water, sediment and soil. No relevant differences between the substances can be seen.

Table 37. Step 2 and Step 3 contributions to the Regional PEC values

Plasticiser	Protection target	Regional PEC (mg/L or mg/kg)		Risk Characterisation Ratio (RCR)		Contribution (%)	
		Step 2	Step 3	Step 2	Step 3	Step 2	Step 3
DEHP	Fresh water	2.60E-04	1.40E-06	13.71	0.075	99.46	0.54
	Sediment (freshwater)	7.10E+01	3.90E-01	0.714	< 0.01	99.46	0.54
	Agricultural soil	5.60E-02	5.50E-06	< 0.01	< 0.01	99.99	0.01
ATBC	Fresh water	2.70E-03	1.70E-05	0.124	< 0.01	99.4	0.6
	Sediment (freshwater)	9.80E+00	5.90E-02	0.235	< 0.01	99.4	0.6
	Agricultural soil	9.00E-03	3.80E-05	< 0.01	< 0.01	99.58	0.42
DEHA	Fresh water	1.50E-03	8.30E-06	18.44	0.104	99.44	0.56
	Sediment (freshwater)	1.00E+01	5.90E-02	1.261	< 0.01	99.44	0.56
	Agricultural soil	5.50E-02	5.40E-06	0.064	< 0.01	99.99	0.01
DEHT	Fresh water	4.60E-04	2.60E-06	5.764	0.033	99.43	0.57
	Sediment (freshwater)	2.50E+01	1.40E-01	2.988	0.017	99.44	0.56
	Agricultural soil	7.00E-02	4.10E-04	46.68	0.273	99.42	0.58
DINCH	Fresh water	1.80E-04	1.20E-06	80.34	0.544	99.33	0.67
	Sediment (freshwater)	1.40E+02	9.50E-01	1.64E+03	11.07	99.33	0.67
	Agricultural soil	2.70E-01	1.50E-03	< 0.01	< 0.01	99.47	0.53
ESBO	Fresh water	2.40E-07	2.10E-09	113.6	1.013	99.12	0.88
	Sediment (freshwater)	4.80E+02	4.30E+00	4.77E+03	42.52	99.12	0.88
	Agricultural soil	7.80E+01	7.70E-03	12.47	< 0.01	99.99	0.01

For the local PEC values, it can be concluded from the Chemical Safety Reports that

- Local PEC values resulting from Step 2 activities are only weakly impacted by Step 3 activities. Releases from Step 2 activities are too low and too widespread to have a significant influence.
- Local PEC values resulting from Step 3 activities are impacted by Step 2 activities in that they are increased by a factor of 10 for surface water and sediment, while the compartment soil shows also here a marginal increase.

2.3.3.4 ConsExpo

2.3.3.4.1 Methodology

ConsExpo contains a secondary exposure model that calculates the exposure to compounds from packaging material via food. The migration of the compound into the food is calculated from the concentration of the compound in the packaging material, the contact area of the packaging and the food and the initial migration rate. The oral exposure resulting from food consumption is subsequently calculated by assuming that the migrated compound is homogeneously distributed over the food and that the intake of the compound is therefore proportional to the fraction of packaged food consumed.

The information with regards to the chemical and the product needed as input in ConsExpo are as defined in Table 38.

Table 38. ConsExpo input data for the Consumer Exposure estimation

	Name	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Substance	CAS number	117-81-7	77-90-7	103-23-1	6422-86-2	166412-78-8	8013-07-8
	Molecular weight (g/mol)	390.56	402.5	370	390.6	424.6	974.7
	LogKow	7.5	4.86	8.94	8.34	10	6.2
Product	Name	Gasket	Gasket	Gasket	Gasket	Gasket	Gasket
	Weight fraction substance (%)	35.8	37.2	34	36.5	37.8	38
Population	Name	general	general	general	general	general	general
	Body weight (Kg)	60	60	60	60	60	60

If the migration rates are not available to estimate the release of the substance from the packaging material, the scenario option 'instantaneous' in Table 39 can be selected to describe the release of all the substance at once.

Table 39. ConsExpo Exposure Scenario data for the exposure estimation of food contact material

Exposure Scenario						
Model: Migration from food packaging						
Substance	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**ESBO**	**DINCH**
Loading	Instantaneous					
Substance concentration (g/cm³)	358	468	340	365	380	378
Thickness packaging (mm)	0.22	0.22	0.22	0.22	0.22	0.22
Contact area (cm²)	15.2	15.2	15.2	15.2	15.2	15.2
Packaged amount (g)	500	500	500	500	500	500
Ingested amount (g/day)	500	500	500	500	500	500

2.3.3.4.2 Results and discussion

The results in Table 40 using the instantaneous release option from the "Migration from food packaging "model gives as result very high levels of daily exposure in comparison with the Tolerable Daily Intake (TDI).

Table 40. Estimated daily intake

	ATBC	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
External dose on day of exposure (mg/kg bw/day)	2.6	1.9	2.0	2.0	2.1	1.9
TDI (mg/Kg bw/ day)	1	0.3	5E-2	1	1	1
Risk Characterization Ratio (RCR)	2.6	6.3	40	2	2.1	1.9

The predictions are very conservative and only take into consideration 3 parameters of the plasticisers: molecular weight, Log Kow and the concentration in the FCM.

The use of a less conservative and more realistic tool/model could be recommended for this application. ConsExpo provides the possibility of a more accurate exposure estimate if information on the migration rate and storage time are available using the 'constant rate' option.

2.3.3.5 Vermeer FCM

2.3.3.5.1 Methodology

Vermeer FCM is a software that allows modelling the migration of chemicals from FCM into food and to predict several toxicological endpoints relevant for FCM compounds. The software was developed within the LIFE VERMEER[26] project and its version 4.0 is included in the MERLIN-expo tool[27].

The migration model input parameters are divided in four blocks:

1. Parameters describing the geometry of the system (Table 41). These parameters are specific to the case and therefore must be known and added manually by the assessor.

Table 41. Parameters describing the geometry of the system

Gasket lid parameters	**Value**
Contact area between FCM and Food (cm^2)	15.19
Density of FCM (g/cm^3)	0.833
Thickness of FCM (cm)	0.022
Volume of Food contained (cm^3)	500

2. The migration model is based on three main processes: the diffusion between FCM and Food, the diffusion coefficient of the FCM and the partition between FCM and Food[28]. These parameters are considered in the second block for the characterisation of the diffusion in the FCM. The Vermeer tool provides the possibility of calculating them using the models or adding measured values.
3. Parameters describing the chemical. The Vermeer tools includes in this section the possibility of using the VEGA tool to predict the Kow values for the chemicals. The QSAR model available for this is the LogP model (MLogP) and the predicted values are presented in Table 42.

Table 42. Parameters describing the chemical

	ATBC	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
Initial concentration of the chemical in FCM (mg/kg)	3.72E5	3.4E5	3.58E5	3.65E5	3.78E5	3.8 E5
Molar mass of the migrating chemical (g/mol)	402	370	390.56	390.6	424.6	974.7
LogKow	2.665	4.737	5.426	5.426	5.183	5.207

4. Parameters characterising the food. These parameters are already included in the tool for chocolate, clear drinks, dry pasta, milk, olive oil, orange juice, tomato sauce and yoghurt (Table 43). Additional foods and their parameters can be included manually.

Table 43. Parameters characterising the food

	Chocolate	**Clear drinks**	**Dry pasta**	**Milk**	**Olive oil**	**Orange juice**	**Tomato sauce**	**Yoghurt**
Density of food (g/cm^3)	0.5	1	0.55	1	0.91	1	1	1.1
Food Ethanol equivalent	70	20	35	60	95	40	25	50

The packaging conditions that most affect migration are the time and temperature of contact. A temperature cycle along the time that the food is in contact with the FCM can also be defined in the Vermeer tool (Table 44).

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[26] Available at: https://www.vegahub.eu/portfolio-item/vermeer-fcm

[27] Available at: https://merlin-expo.eu/download-merlin-expo/

[28] Vermeer use manual available at: https://merlin-expo.eu/wp-content/uploads/2022/04/VERMEER-FCM-Manual-v3.4.pdf

Table 44. Packaging conditions

Process	**Time**	**Temperature (°C)**
Sterilisation	30 min	85
Storage, unopened	6 months	20
Storage, opened	2 months	-18

The tool includes information with regards to the Specific Migration limits of chemicals and Group Specific Migration Limits (SML(T)) in Annex 1 of Regulation 10/2011. This information can be manually added as well (Table 45).

Table 45. Specific migration limits

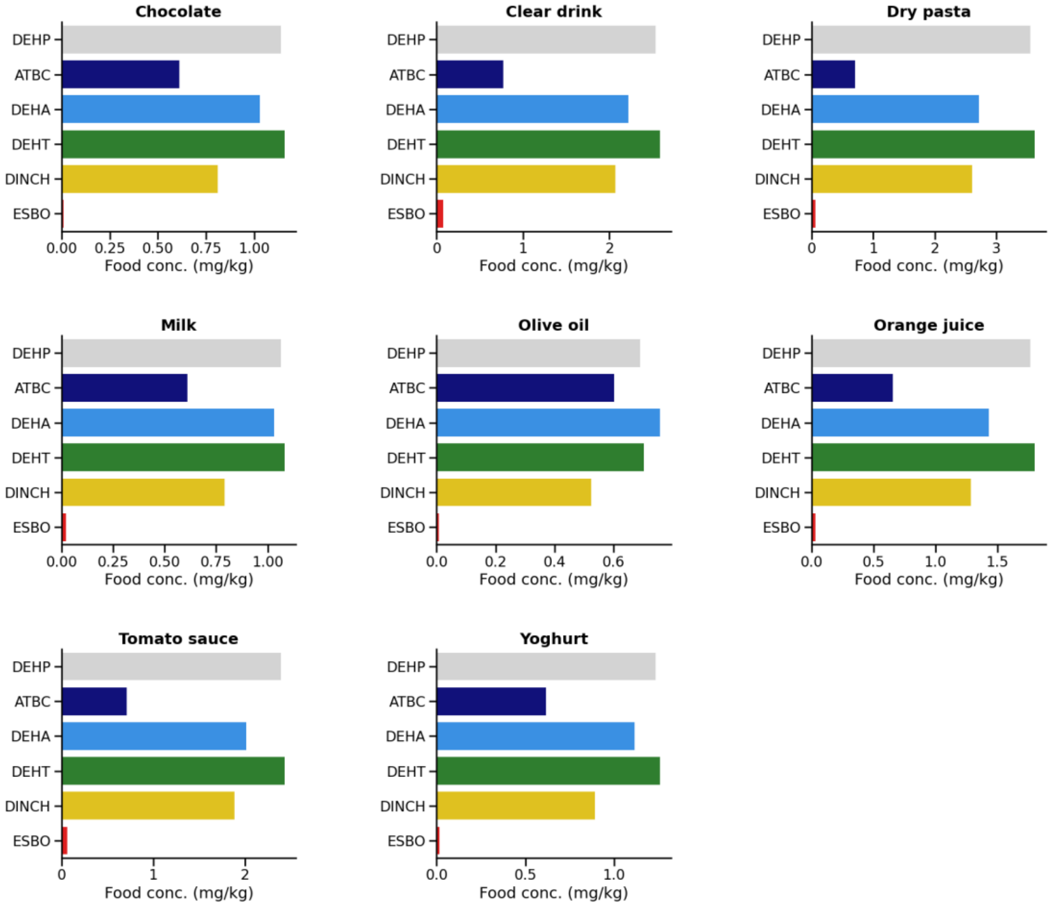
	ATBC	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
SML (mg/kg)	-	18	1.5	60	-	60
SML(T) (mg/kg)	60	60	60	60	60	60

2.3.3.5.2 Results and discussion

The most relevant outputs of the migration model in the Vermeer FCM software are the Concentration of the plasticisers in the food at a given time and the ratio between the concentration and the specific migration limit.

Figure 11 graphs illustrate the concentration of each individual plasticiser in the different food systems.

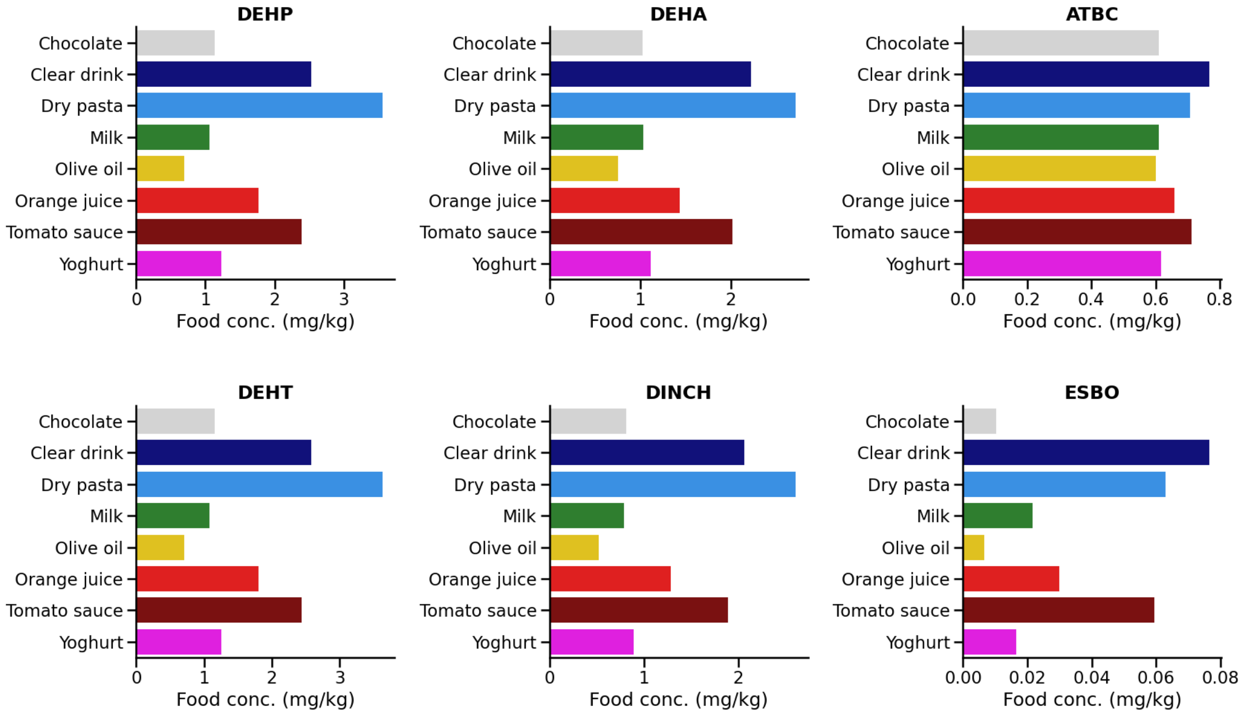
Figure 11. Concentration of plasticiser in all food systems



Dry Pasta seems to be the food system in which most of the plasticisers investigated - with the exception of ESBO and ATBC - migrate more, followed by clear drinks, tomato sauce and orange juice. ESBO and ATBC migrate faster in clear drinks, but the other systems are the same. These systems are the lowest food-Eth equivalence.

Figure 12 illustrates the concentration of all plasticisers for the same food systems.

Figure 12. Concentration of plasticiser per food system



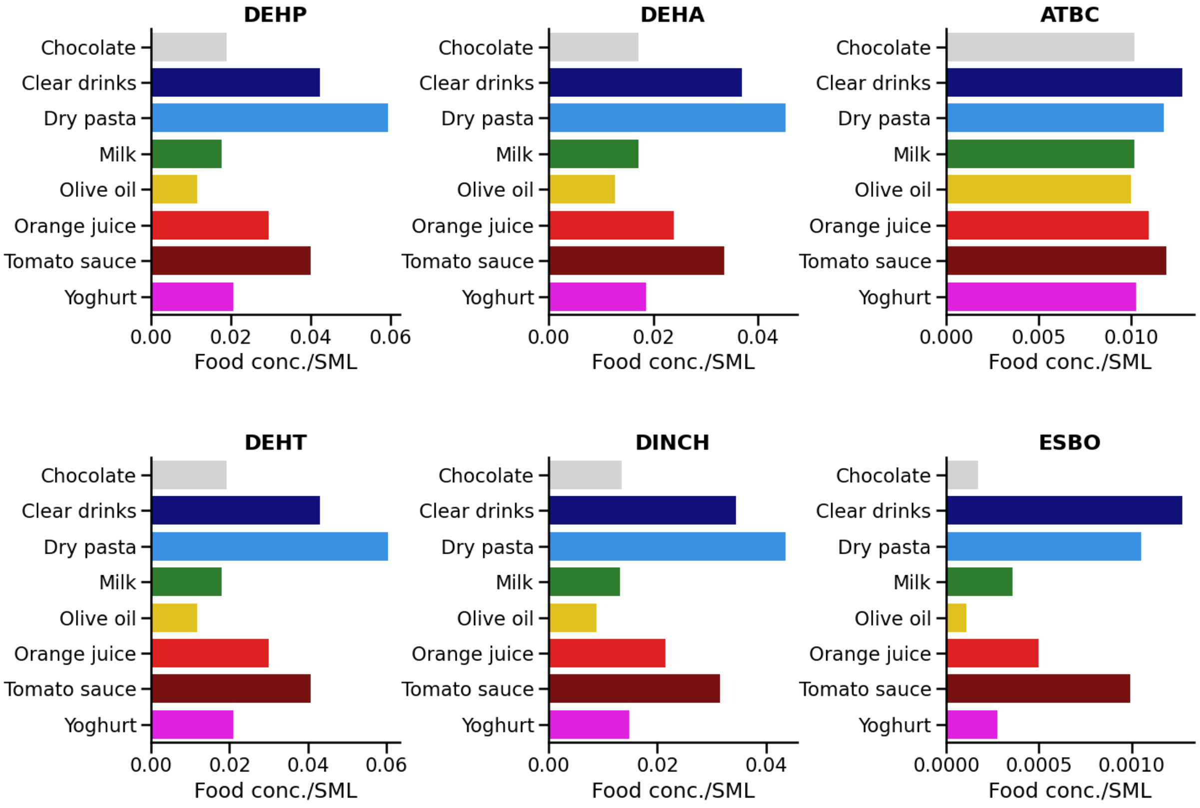
Analysing these results, it is evident that for all the food systems, except olive oil, DEHT - closely followed by DEHP - are the plasticisers that migrate more. These are followed by DEHA and DINCH being the less migrating plasticiser ATBC and ESBO in this order. The exception is olive oil where DEHA is the plasticiser that migrates the most.

The effect of the molecular weight of the plasticiser can be seen in these results. The lower the molecular weight, the larger its diffusion into the food and vice versa. In this case ESBO is by difference the plasticiser with the higher molecular weight and the one that migrates the less in all the food systems.

The octanol-water partitioning coefficient (Kow) is another parameter that reflects the capacity for migration and can be seen in the graphics in Figure 13. Kow represents the lipophilicity of the migrant. The higher is the Kow, the more lipophilic and therefore the more migration can be expected, given that the food has a high fat content. In this case, ATBC is the plasticisers that has the lowest predicted Kow and the second plasticiser that migrates the less.

Figure 13 illustrates the ratio between the concentration and specific migration limit concentration of each individual plasticiser in the different food systems

Figure 13. Ratio between concentration and the SML per plasticiser



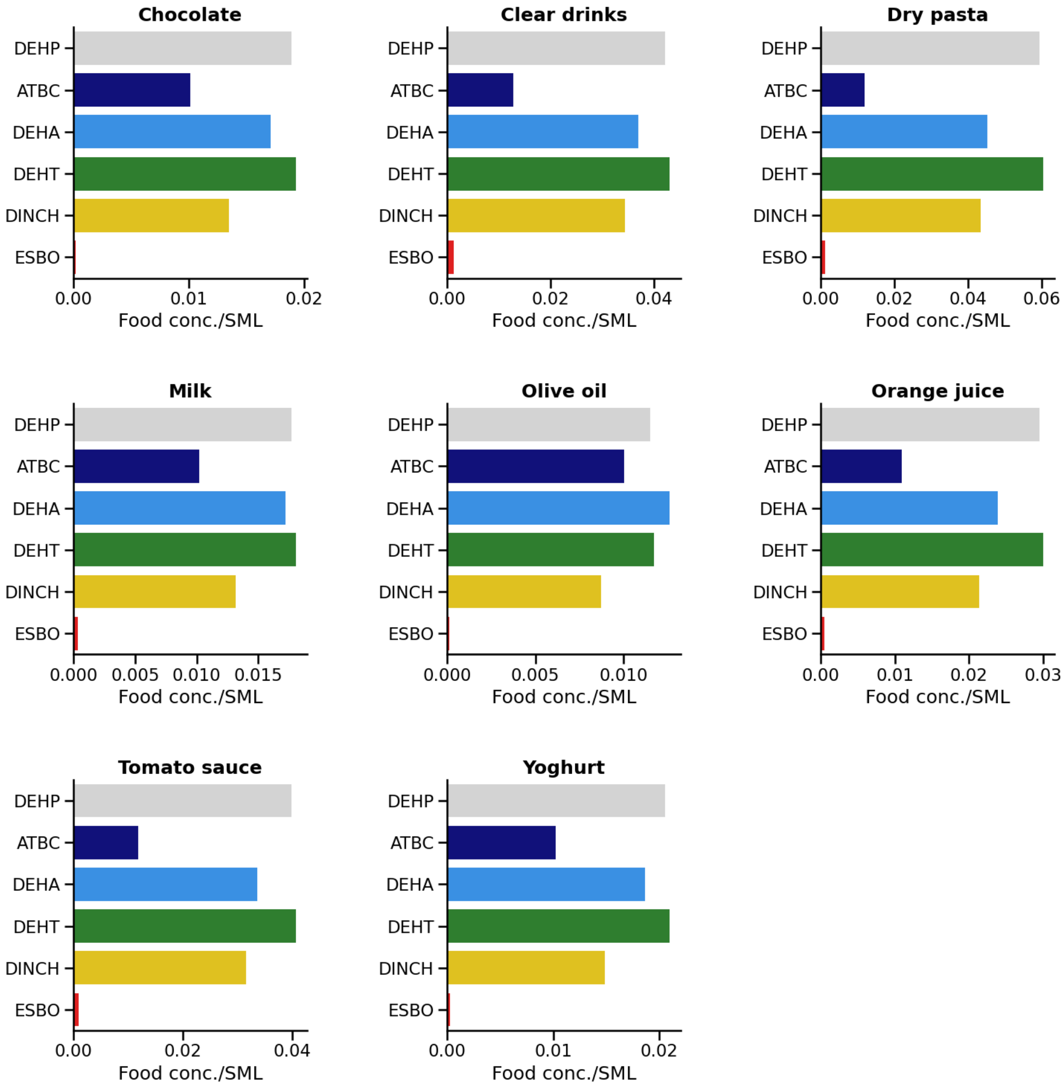
For most of the plasticisers the ratio between the concentration and SML goes from the highest to the lowest in the following food systems: Dry pasta>clear drinks>tomato sauce>orange juice>yoghurt>chocolate>olive oil. The exception is ATBC which also shows a more similar trend and values for all the food systems.
Figure 14 illustrates the ratio between the concentration and SML concentration of all the plasticisers for the same food systems. The highest values for the ratios between the concentration and the SML are for DEHP followed by DEHA. These are the two chemicals with the lowest SMLs.

Using the data of the plasticiser in the olive oil food system a migration rate has been estimated for each plasticiser to be used as input data in ConsExpo and run the 'constant rate' option of the model (Table 46).

Table 46. ConsExpo Exposure Scenario data for the exposure estimation of FCM

Exposure Scenario						
Model: Migration from food packaging						
Substance concentration	**ATBC**	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
Loading	Constant rate					
Substance concentration (g/cm^3)	0.468	0.340	0.358	0.365	0.378	0.380
Thickness packaging (mm)	0.22	0.22	0.22	0.22	0.22	0.22
Contact area (cm^2)	15.2	15.2	15.2	15.2	15.2	15.2
Packaged amount (g)	500	500	500	500	500	500
Ingested amount (g/day)	500	500	500	500	500	500
Migration rate (mg/day)	4.6E-3	5.4 E-3	5.0 E-3	5.0 E-3	4.0 E-3	4.33E-5
Storage time (months)	8	8	8	8	8	8

Figure 14. Ratio between the concentration and specific migration limit (SML) per food system



The results using the constant rate release option from the "Migration from food packaging "model provide more realistic results (Table 47).

Table 47. Exposure estimation and risk characterisation

	ATBC	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
External dose on day of exposure (mg/kg bw/day)	1.9E-2	2.0E-2	2.0E-2	2.0E-2	1.6E-2	1.8E-4
TDI (mg/kg bw/day)	1	0.3	0.05	1	1	1
Risk Characterization Ratio (RCR) (mg/kg)	1.9E-2	6.0E-3	4.0 E-2	2.0E-2	1.6E-2	1.8E-4

2.3.3.6 Scoring

The indicators and criteria to define the safety levels in Step 3 will be very specific to the final application. These might differ for each case depending on the assessment requirements in the specific product legislation.

In order to capture this possibility, a different scoring system that follows the proposal in Table 6 of the SSbD framework (Caldeira et al., 2022b) is considered for this step (Table 48).

The scoring proposed is based on the results obtained with the Vermeer tools.

Table 48. Scoring system proposed

Risk Characterization Ratio (RCR)	SSbD Step 3
> 1.5	**0**
1.1-1.5	**1**
0.5-1	**2**
<0.5	**3**

The results are presented for the six plasticisers per food system in Table 49.

Table 49. SSbD scoring for Step 3

	Chocolate	Clear drinks	Dry pasta	Milk	Olive oil	Orange juice	Tomato sauce	Yogurt
DEHP	2	0	0	2	3	1	0	2
ATBC	3	3	3	3	3	3	3	3
DEHA	3	3	3	3	3	3	3	3
DEHT	3	3	3	3	3	3	3	3
DINCH	3	3	3	3	3	3	3	3
ESBO	3	3	3	3	3	3	3	3

2.3.3.7 Conclusions for step 3

The difference in the results applying different tools illustrates the complexity of the assessment of FCMs. The prediction of the migration of the chemicals from FCM to food and especially from soft PVC is shown to be challenging. Many different factors need to be considered for which no experimental data is available and therefore modelling is not possible.

The importance of the availability of data to predict the exposure is demonstrated when applying the two different loadings in ConsExpo.

From the input data needed for the simulation and the detailed results provided, the Vermeer tool seems to provide the most thorough assessment, although it still uses default values for the PVC FCMs when simulating the migration of chemicals from this polymer matrix.

In all the approaches, a very conservative FCM scenario is applied considering that the entire metal closure is covered by the plastisol liner and that the plastisol is always in contact with the food. This again demonstrates the importance of data for the development of a more realistic FCM scenarios and the prediction of plasticisers' migration.

2.3.4 Step 4 Environmental sustainability assessment

This step covers the assessment of the environmental sustainability aspects of the plasticiser, with a specific focus on environmental impacts along its entire life cycle, from extraction of raw materials up to waste management. This is done by means of life cycle assessment (LCA), conducted for the six plasticisers in the application of a gasket manufacturing for metal cap. The Environmental Footprint (EF) method has been applied. The EF is the Commission's recommended method to assess the environmental performance of products (EC, 2021a). The EF method presents the classical 4 LCA steps: goal and scope, life cycle inventory, life cycle impact assessment, and interpretation. The goal and scope of the study are presented in section 2.3.4.1, the inventory is described in section 2.3.4.2, and the life cycle impact assessment is presented in section 2.3.4.3. The interpretation and data quality assessment are reported in Annex 8. As indicated in the proposed SSbD framework, a method for absolute environmental sustainability assessment (AESA) is also applied being the results presented in section 2.3.4.4.

2.3.4.1 Goal and Scope

The scope of the LCA is to compare different gaskets in a food contact application, manufactured using alternative plasticisers, and to investigate which data are required and their influence on the application of LCA in the SSbD context.

2.3.4.1.1 Functional unit and reference flow

The functional unit defines the quantitative and qualitative aspects that a product under assessment should provide. According to the product environmental footprint (PEF) method (EC, 2021) the functional unit shall be described considering the following aspects:

- The function(s)/service(s) provided: "**what**";
- The extent of the function or service: "**how much**";
- The expected level of quality: "**how well**";
- The duration/lifetime of the product: "**how long**";

The functional unit of this study is based on the function of the product in which the plasticiser is used. The SSbD framework should be applied considering a specific application and consider the entire life cycle of the chemical. This is aligned with the PEF method that requires that, for comparability among products, the function should be such that it covers the entire life cycle. As already presented, the product selected is a gasket for metal caps, being the functional unit of the gasket to provide an airtight seal (what) between one glass jar and its metal cap (how much), able to last for the whole shelf-life of the food content of the jar (how long), and which is suitable for the contact with oily food (how well).

The reference flow is defined as the amount of product required to achieve the functional unit. In this case, the reference flow is one kg of PVC gaskets. The choice of the plasticiser does not influence the dimension and weight of the gasket, hence, it is possible to define the reference flow as the amount of gaskets expressed in mass. The plasticiser choice will influence the composition of the gasket. Table 3 (section 2.1.2.2) shows a summary of the composition of the different formulations used, each of them including a different plasticiser.

It is important to highlight that the function of the gasket is tightly linked to the function of the plasticiser since the main purpose of the plasticiser is to modify the properties of the PVC and to meet the technical requirements for the gasket.

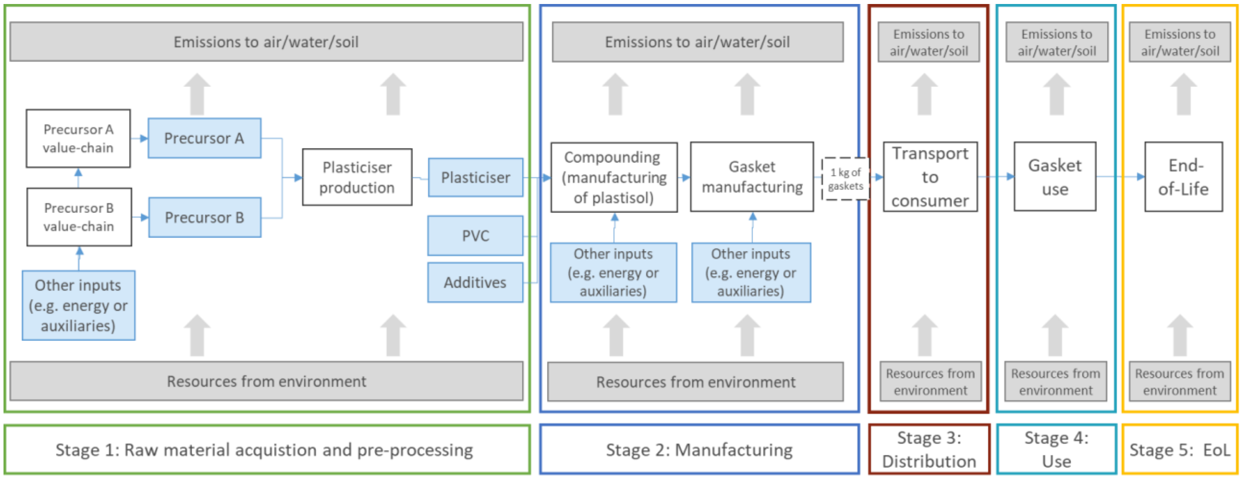
2.3.4.1.2 System boundaries

The study follows a cradle-to-grave approach, so the system boundaries encompass: the supply-chain of the raw materials used for the manufacturing of the gasket (plasticisers, PVC, and additives), all the steps required for the gasket manufacturing (compounding, gasket application and curing), the distribution to the consumer, the use of the gasket, and its final disposal after the consumption of the food inside the jar. Figure 15 shows a graphical representation of the system boundaries for step 4.

2.3.4.1.1 Environmental Footprint impact categories

As described in the SSbD framework, the impact categories of the EF method were considered, which includes 16 environmental impact categories (presented in Table 51, and in more detail, in Annex 8). The method includes human toxicity (cancer and non-cancer) and ecotoxicity impact categories that relate to the main goal of SSbD, aiming at the identification of chemicals that help moving towards a 'toxic-free environment'. These impact categories differ from the assessment conducted in Step 3 as they refer to impacts due to all chemicals being emitted along the product life cycle, which ultimately may impact humans and the environment via environmental compartments (e.g. soil, water, air). The focus of the assessment is rather on indirect impacts via different compartments (the so-called residual toxicity) and in the overall toxicity footprint rather than a specific focus on direct exposure, which is addressed in previous evaluation steps of the SSBD framework. These toxicity related impact categories rely on the underlying multimedia box model embedded in USEtox, i.e. address also the transfer of chemicals from one compartment to the other due to environmental conditions and the specific physicochemical properties of the chemicals which are assessed.

Figure 15. Life cycle stages included in the study according to PEF method



The different impacts categories were clustered in 4 groups: toxicity, climate change, pollution, and resources, reflecting LCA assessment levels that relate to different policy objectives, as presented in (Caldeira et al., 2022b).

The EF method version 3.1 was used. The case study was run with the Simapro software.

2.3.4.2 Life Cycle Inventory

The life cycle is divided in stages following the standard division used in the PEF method, as anticipated in the goal and scope. The life cycle stages include:

- Raw material acquisition and pre-processing (including production of plasticiser PVC and other chemical substances included in the composition of the gasket);
- Manufacturing (production of the plastisol and the gasket);
- Distribution (transport of the gasket to final customer);
- Use stage;
- End-of-life (including the disposal of the gasket).

Figure 15 shows the life cycle stages for a generic plasticiser, assuming that the production, the use and the end-of-life are happening in Europe. To model the life cycle inventory, the following data are usually needed to be collected for each stage of the life cycle:

- Raw materials consumption
- Energy and water consumption
- Ancillary materials consumption used for the production
- Air, water, soil, and waste emissions
- Transportation of the raw materials

The source of the data is strictly related to the data availability. Primary data are site-specific and they need to be collected for the processes directly controlled by the organization that is developing the LCA, and when possible, the processes directly controlled by the suppliers. Secondary data are usually not site-specific and they are collected for all the processes not directly controlled by the LCA practitioner (i.e. raw material acquisition). Usually, database are used to model all the processes where data are not available. If no datasets are available, proxy data or data from literature can be used to complement the inventory analysis. In the case study, dataset from ecoinvent v3.6

(Wernet et al. 2016) were used, complemented with data retrieved from literature. Annex 7 shows the detailed life cycle inventory for each stage of the life cycle.

Box 1. Circularity in the PEF method

Circularity in the PEF method

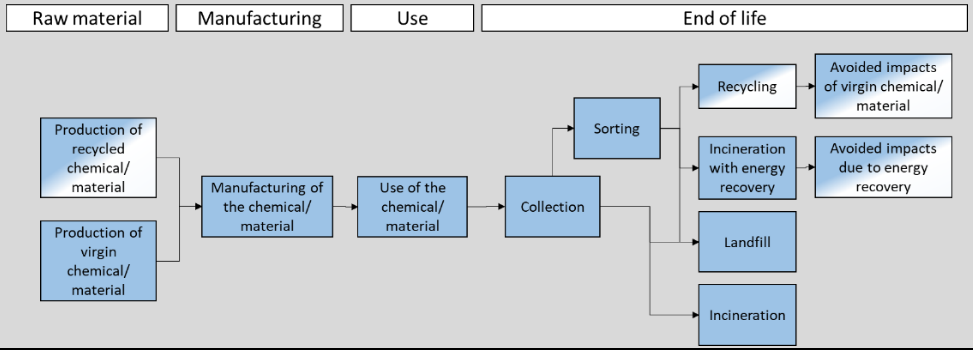
An important aspect to consider in the SSbD is the circularity of the chemical/material system. In the SSbD framework, several indicators for circularity are suggested to be considered in the design phase. However, as Caldeira et al. (2022b) pointed out, the adherence to such principles does not allow to conclude on the sustainability performance of the chemicals and materials, and the safety and sustainability assessments should be conducted. Most of the circularity metrics positively account for the high recycled content, regardless specifying the recycled material and its recycling process, or for the use of biomass feedstock, without distinguishing the different impacts of the types of biomass. This may lead to burden-shifting between different impact categories.

LCA is able to cover also aspects of the circular economy, such as the recycling of the chemical/material at the end-of-life, the energy recovery from the waste treatment, and the use of recycled feedstock. These aspects are defined in the goal and scope when setting the system boundaries. LCA allows for a deeper analysis of the benefits of the circular economy, since it quantifies impacts across different environmental impact categories, rather than attribute an absolute positive value to a single circularity metric.

In this direction, the Circular Footprint Formula (CFF) has been developed in the PEF method to quantify these impacts, and allocate the burdens of the waste production and recycling treatment along the different life cycles. Indeed, the recycling process has two functions: on one hand, the production of a recycled material (also as secondary raw material), and on the other hand, the waste treatment. Therefore, the impacts could be shared between the life cycle producing and treating the waste, hence using the waste treatment as service, and the subsequent life cycle of a product using the recycled material, hence using the recycled material production as service.

The CFF includes the effect of change in performances delivered by the recycled material compared to the virgin one and a parameter to allocate the burdens across the system that is producing the waste and the one using the recycled material, taking into account the specific market situation of the secondary material. For energy recovery it follows the system expansion approach, to include avoided production of the energy substituted with the incineration activity.

Figure 16. Life cycle of a generic product. The shaded boxes represent processes for which the impacts can be allocated between the adjacent product life cycles, according to chosen modelling approach



2.3.4.3 Life Cycle Impact Assessment results

The results of the LCA are used to derive the SSbD score as proposed in (Caldeira et al., 2022b). The score for each impact category reflects the degree of improvement relatively to the reference gasket (the DEHP). The proposed thresholds of improvement have been updated compared to the previous proposal to differentiate similar performances from a worsening. Therefore, the **scores that were attributed to each impact category as <u>illustrative</u>** are: “0” when the alternative presents impacts 10% higher than the reference, “1” when results from the alternative are from 10% higher to 5% lower, “2” when results of the alternative are 5% lower to 10% lower, and “3” when results of the alternative are 20% lower or more as presented in Table 50. **It is important to note that this scoring system is not definitive, and it has an illustrative purpose only. This will be further developed with the testing phase.**

The improvements are calculated as follow:

$$Improvement\ (\%) = \frac{I.C._{ref}^{a} - I.C._{alt}^{a}}{I.C._{ref}^{a}}$$

In which I.C. $^{a}_{ref}$ refers the impact category value of the reference gasket (DEHP), whilst I.C. $^{a}_{alt}$ is the value of the same impact category of the alternative gasket.

Table 50. Scoring for step 4

Improvement (%)	Score for impact categories
<= -10%	0
-10% - +5%	1
+5% - +20%	2
>20%	3

The sixteen impact categories are grouped in 4 levels: Toxicity (E1), Climate change (E2), Pollution (E3) and Resources (E4). A level is considered achieved when the chemical scores at least 2 in all the impact categories of that level. The result of such assessment is presented in Table 51. Based on proposed the calculation methodology of the score, ATBC and DEHA do not show any improvement relatively to DEHP. DEHT performs slightly better for all impact categories except for Resources, mineral and metals, though no level is passed. In the case of DINCH except for Climate Change, Land use, Resource use, fossil and Ionizing radiation it has the highest score, which means a large improvement when compared with the reference. Furthermore, it passes the level of toxicity, which is not achieved by any other gasket. Finally, ESBO shows a higher score, with a large improvement on the Resource use, fossil, and also for some categories of the pollution level. On the other hand, it does not show any improvement for about half of the categories.

Table 51. Scores obtained for each of the alternative gaskets in the different impact categories

LEVEL	IMPACT CATEGORY	SSbD SCORES											
		DEHP		ATBC		DEHA		DEHT		DINCH		ESBO	
Toxicity E1	Human toxicity, cancer	1	X	0	X	0	X	1	X	2	V	0	**X**
	Human toxicity, non-cancer	1		0		1		1		2		1	
	Ecotoxicity, freshwater	1		0		1		1		2		1	
Climate Change E2	Climate change	1	X	1	X	0	X	1	X	1	X	0	**X**
Pollution E3	Ozone depletion	1	X	1	X	1	X	1	X	2	X	2	**X**
	Particulate matter	1		0		0		2		2		2	
	Ionizing radiation, human health	1		1		1		1		1		2	
	Photochemical ozone formation, human health	1		0		1		2		2		2	
	Acidification	1		0		0		1		2		2	
	Eutrophication, terrestrial	1		0		0		1		1		1	
	Eutrophication, freshwater	1		0		1		1		2		1	
	Eutrophication, marine	1		0		0		1		2		0	
Resources E4	Water use	1	X	0	X	1	X	1	X	1	X	1	**X**
	Land use	1		0		1		1		2		0	
	Resource use, fossil	1		1		1		1		1		3	
	Resource use, minerals and metals	1		0		0		1		2		0	
PASSED LEVELS				**0**		**0**		**0**		**1**		**0**	

The results of the impact assessment are presented at the characterisation level in Figure 17. Additionally results of step 4 are also presented and interpreted according to the requirements of the PEF method in Annex 8. The interpretation of LCA results following the PEF can be used to understand where the environmental performances of the chemical/material can be improved, both at life cycle stage, and at impact category level and which needs to be improved. This information can be used in the re-design of a chemical/material production process.

Figure 17. Cradle to grave characterized results of the sixteen impact categories of the environmental footprint for 1 kg of each gasket

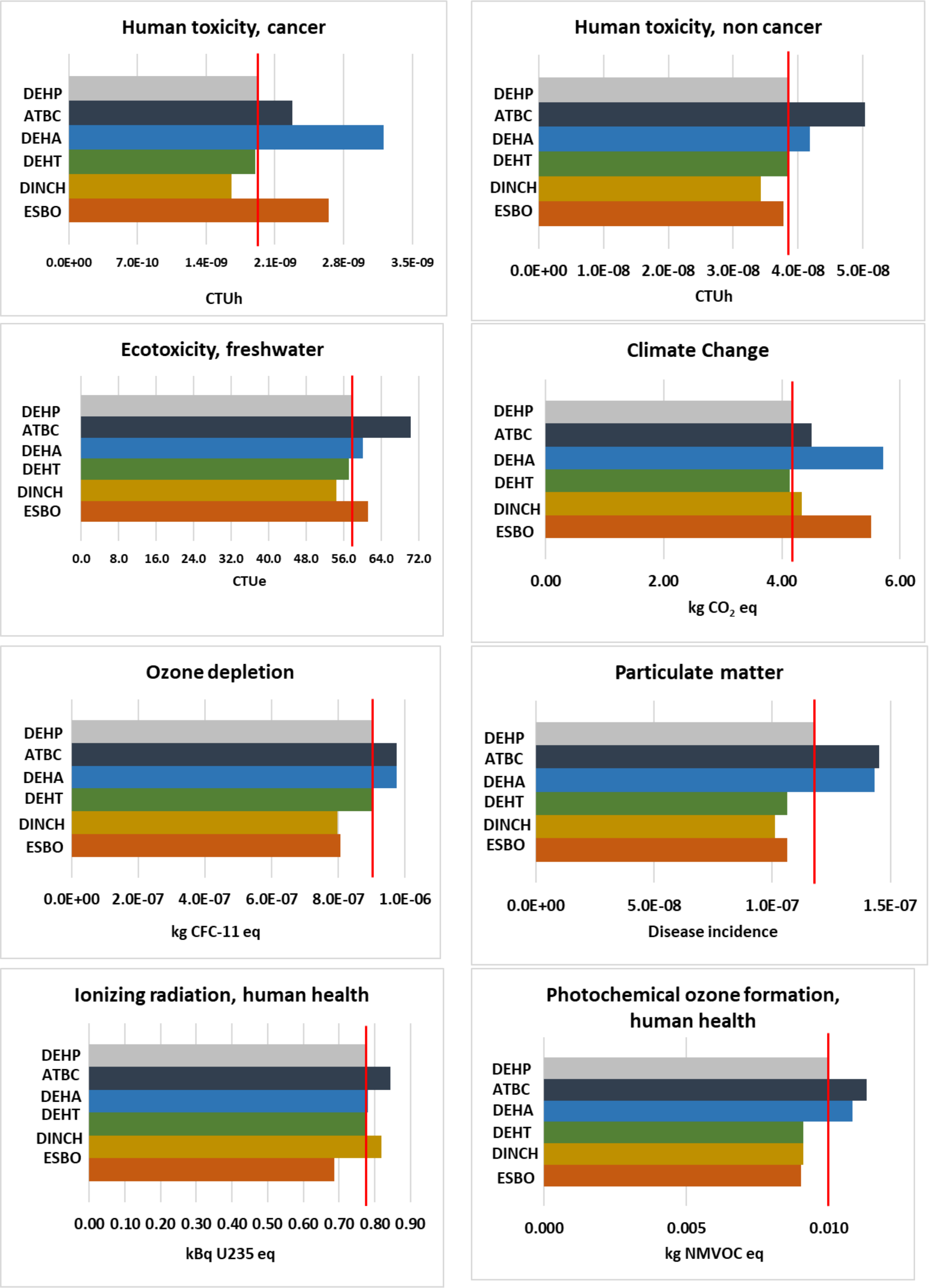
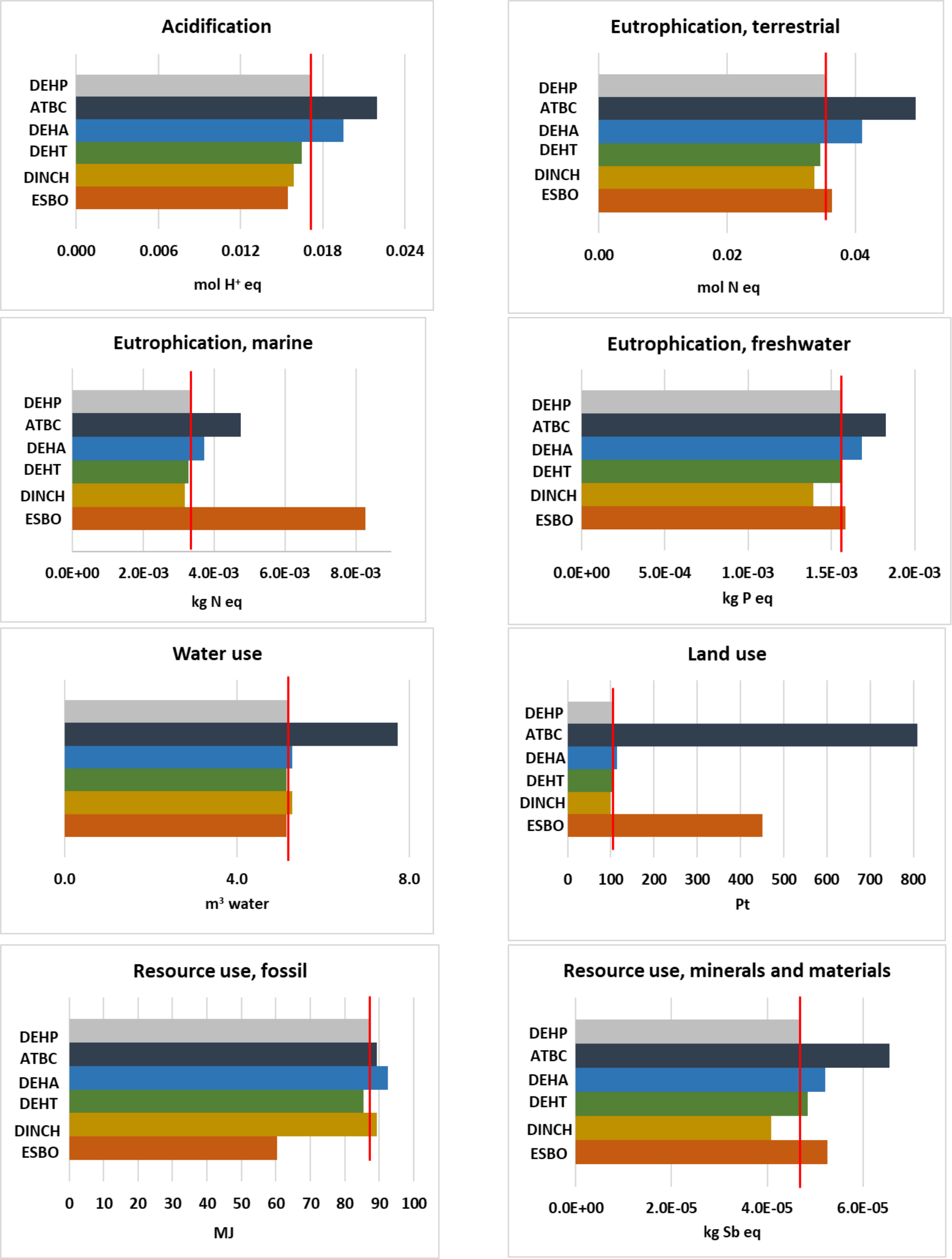


Figure 17 Cradle to grave characterized results of the sixteen impact categories of the environmental footprint for 1 kg of each gasket (continuation)



2.3.4.4 Illustration of how LCA results can support the re-design of a chemical/material

In the (re)-design phase of the SSbD framework, several principles and indicators are proposed to support the design of new chemicals/materials or the re-design of existing ones. The case study developed the assessed chemicals are already established products in the plasticisers industry, therefore a redesign and optimisation of the chemical life cycle can be explored.

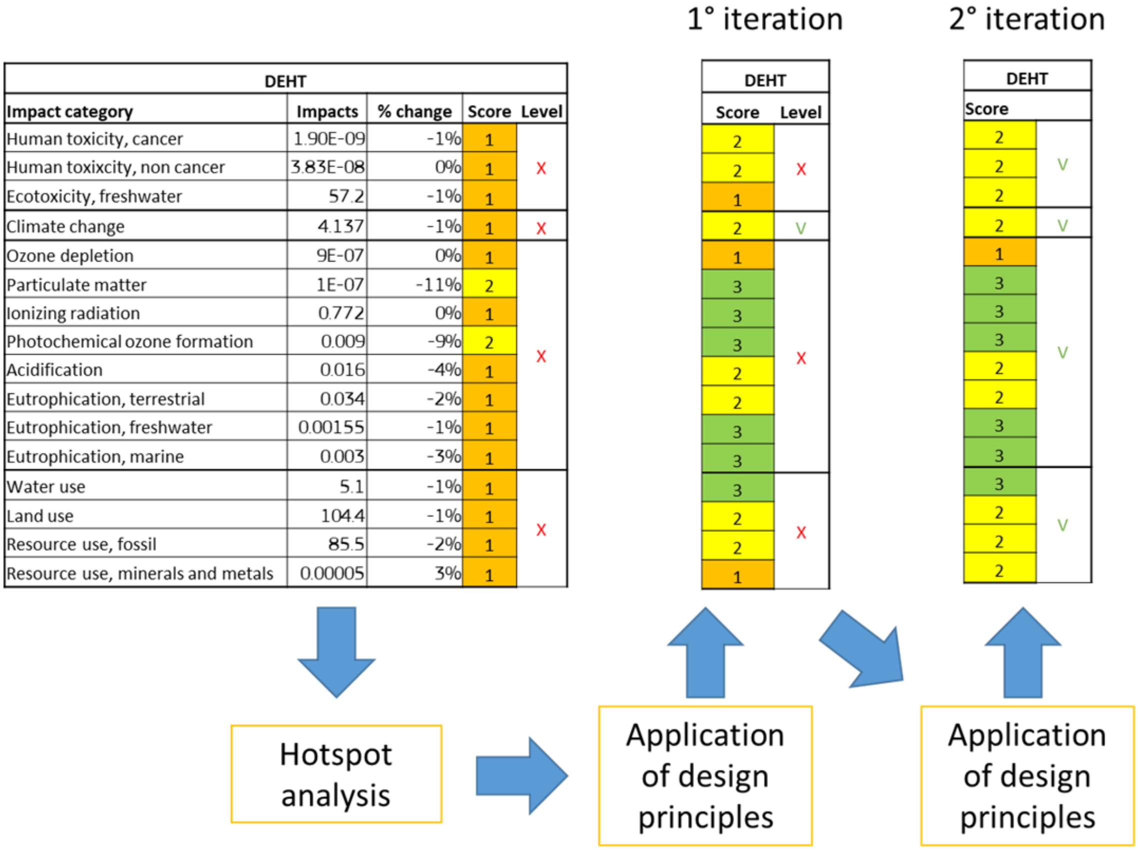
For example, DEHT exhibits overall scores of 1 and so one can explore further improving of some processes to see if a re-design of the processes would increase the environmental profile of DEHT to score above 2. Since the category resource depletion, mineral and metals is the farthest from the target, as shown in Table 50, it is important to detect the processes that contribute the most to the impact category. However, some can be under the direct control of the organization assessing the chemical and may be easier to address, other may involve background processes that the organization/assessor cannot directly control or influence.

Regarding this impact category, the most relevant processes are shown in Annex 8 Table A52. The production of terephthalic acid along with other ones concerning other components of the gasket, such as the PVC and the additives, or the manufacturing stage, such as the electricity. So, an example of possible re-design initiatives can be:

- To **refine the current LCA model** (e.g. specific energy consumption and fuel mix used) by engaging with the supplier of terephthalic acid to verify if a specific LCA for this chemical is available or if they are willing to share information through data collection. Then, the assessment can be updated to show any relevant change to the environmental profile. This action will also reduce the uncertainty in the assessment. Additionally, if no reasonable improvements of the environmental profile are observed, other suppliers of terephthalic acid that produce it with other industrial processes (e.g. from oxidation of bio-based xylenes or depolymerisation of waste PET) can be explored by evaluating their environmental performances.
- To explore ways to reduce the environmental impacts of **the processes directly under the control of the organization** (in this case, the plasticiser manufacturer). This can be done by reducing net energy consumption, switching to other types of energy sources, improving the process efficiency, etc. For a given energy mix supplied to the process, it is also possible to use an indicator as the energy consumption per kg of plasticiser to track the improvement. In case more options are available, LCA can also be used to simulate ex-ante improvement in environmental impacts due to different re-design option (e.g. improve energy efficiency of a piece of equipment versus install solar panels to provide part of the electricity needed in the plant).

Figure 18 shows the possible refinement procedure of results for each iteration of the assessment. Starting from the DEHP results obtained initially, further improvement can be put in place focusing on the impact categories that do not perform well. Processes that influence the performance of one impact category should be analysed avoiding the worsening of the other impact categories, namely burden shifting. Involvement of the expert judgment for the results interpretation is needed to support the decision making.

Figure 18. Iterative re-design process. Starting from the first assessment, hotspots are identified and prioritised for improvement. In each iteration the assessment is updated until it meets the SSbD requirements



DEHT				
Impact category	**Impacts**	**% change**	**Score**	**Level**
Human toxicity, cancer	1.90E-09	-1%	1	X
Human toxixcity, non cancer	3.83E-08	0%	1	
Ecotoxicity, freshwater	57.2	-1%	1	
Climate change	4.137	-1%	1	X
Ozone depletion	9E-07	0%	1	X
Particulate matter	1E-07	-11%	2	
Ionizing radiation	0.772	0%	1	
Photochemical ozone formation	0.009	-9%	2	
Acidification	0.016	-4%	1	
Eutrophication, terrestrial	0.034	-2%	1	
Eutrophication, freshwater	0.00155	-1%	1	
Eutrophication, marine	0.003	-3%	1	
Water use	5.1	-1%	1	X
Land use	104.4	-1%	1	
Resource use, fossil	85.5	-2%	1	
Resource use, minerals and metals	0.00005	3%	1	

1° iteration

DEHT	
Score	**Level**
2	X
2	
1	
2	V
1	X
3	
3	
3	
2	
2	
3	
3	
3	X
2	
2	
1	

2° iteration

DEHT	
Score	
2	V
2	
2	
2	V
1	V
3	
3	
3	
2	
2	
3	
3	
3	V
2	
2	
2	

2.3.4.5 *Absolute Environmental Sustainability Assessment*

The SSbD framework considers as well the use of absolute sustainability assessment methods, as they would allow to consider ecosystems carrying capacities in environmental assessments. In recent years, several methods have been developed linking the Planetary Boundaries (PB) framework to LCA. There is, however, currently no common framework (Bjørn et al., 2019) encompassing all relevant processes and scales. Especially for chemical pollution (relevant for human toxicity and ecotoxicity in SSbD Step 4) and for aerosol loading (relevant for particulate matter impacts in SSbD Step 4), there is no boundary or carrying capacity defined at any relevant spatial scale (Persson et al., 2022), despite initial attempts to develop related methods (e.g. Kosnik et al., 2022) In this case study, we tested two methods, one provides carrying capacity-based normalisation references for the EF midpoint categories (Sala et al., 2020) and it is reported hereunder. Another approach, is based on PB-informed characterisation models defining characterisation factors (CFs) to map the elementary flows onto the control variables (Ryberg et al., 2018, 2021). For consistency the former is presented in the following section as it is applicable to the Environmental Footprint method impact categories. The latter is presented as example of alternative methods for which there is not a direct alignment with the EF impact categories in Annex 9.

2.3.4.5.1 Planetary Boundaries-based normalisation factors

The characterised results can be normalised applying the planetary boundaries based normalisation factors of Sala et al. (2020). This set of normalisation factors is not the one included in the PEF method, but it represents an attempt to link the impact of a product to the global carrying capacities and highlight impact categories which represent hotspot if considered in relation to planetary boundaries.

To identify the most relevant impact categories, the normalised impact for each category (which represents the fraction of carrying capacities used by the reference flow for each impact category) has been divided by the sum of the normalised impacts (which represents the total carrying capacities used by the reference flow). This procedure allows setting up a rule for the identification of most relevant impact categories that is independent from the absolute scale of the impacts. Table 52 shows that the most relevant impact categories identified are six (identified in grey), while the most relevant impact categories identified in Annex 8 were eight (Climate change, Resource use fossil, resource use, minerals and metals, water use, eutrophication, freshwater, ecotoxicity, acidification and land use). Moreover, by using the PB normalization (more detail in Annex 9), Particulate Matter impact category appears as one of the most relevant impact categories, while it was not identified with the EF normalized and weighted results.

Comparing the impacts normalised with the PB-based factors it can be seen that the most relevant categories are also the ones that are globally trespassing the safe operating space (climate change, particulate matter, ecotoxicity, resource use, fossil fuels and minerals and metals, freshwater eutrophication and land use).

Table 52. Planetary Boundaries normalised results (Sala et al., 2020) for the six gaskets (Cradle to grave).

Impact Categories	**ATBC**		**DEHA**		**DEHP**		**DEHT**		**DINCH**		**ESBO**	
	[-]	**[%]**	**[-]**	**[%]**	**[-]**	**[%]**	**[-]**	**[%]**	**[-]**	**[%]**	**[-]**	**[%]**
Climate change	4.6E-03	23.7	5.8E-03	31.6	4.2E-03	26.9	4.2E-03	27	4.4E-03	28	5.6E-03	33
Ecotoxicity, freshwater	3.7E-03	19.2	3.2E-03	17.3	3.0E-03	19.3	3.0E-03	19	2.9E-03	18	3.2E-03	19
Resource use, fossil	2.8E-03	14.3	2.9E-03	15.6	2.7E-03	17.1	2.6E-03	17	2.8E-03	18	1.9E-03	11
Eutrophication, freshwater	2.2E-03	11.3	2.0E-03	10.9	1.9E-03	11.8	1.8E-03	12	1.7E-03	11	1.9E-03	11
Particulate Matter	1.9E-03	10.1	1.9E-03	10.5	1.6E-03	10.0	1.4E-03	9.2	1.4E-03	8.7	1.4E-03	8.3
Resource use, minerals and metals	2.1E-03	10.7	1.6E-03	9.0	1.5E-03	9.4	1.5E-03	9.9	1.3E-03	8.3	1.7E-03	9.7
Water use	2.9E-04	1.5	2.0E-04	1.1	2.0E-04	1.2	2.0E-04	1.3	2.0E-04	1.3	2.0E-04	1.1
Photochemical ozone formation, human health	1.9E-04	1.0	1.8E-04	1.0	1.7E-04	1.1	1.5E-04	1.0	1.5E-04	1.0	1.5E-04	0.9
Land use	1.1E-03	5.6	1.5E-04	0.8	1.4E-04	0.9	1.4E-04	0.9	1.3E-04	0.8	6.0E-04	3.5
Acidification	1.5E-04	0.8	1.4E-04	0.7	1.2E-04	0.8	1.1E-04	0.7	1.1E-04	0.7	1.1E-04	0.6
Eutrophication, marine	1.6E-04	0.8	1.3E-04	0.7	1.2E-04	0.7	1.1E-04	0.7	1.1E-04	0.7	2.8E-04	1.7
Human toxicity, non-cancer	8.5E-05	0.4	7.0E-05	0.4	6.5E-05	0.4	6.4E-05	0.4	5.8E-05	0.4	6.4E-05	0.4
Eutrophication, terrestrial	5.6E-05	0.3	4.6E-05	0.3	4.0E-05	0.3	3.9E-05	0.3	3. 8E-05	0.2	4.1E-05	0.2
Human toxicity, cancer	1.6E-05	0.1	2.3E-05	0.1	1.4E-05	0.1	1.4E-05	0.1	1.2E-05	0.1	1.9E-05	0.1
Ozone depletion	1.3E-05	0.1	1.3E-05	0.1	1.2E-05	0.1	1.2E-05	0.1	1.0E-05	0.1	1.0E-05	0.1
Ionizing radiation, human health	1.1E-05	0.1	1.0E-05	0.1	1.0E-05	0.1	1.0E-05	0.1	1.1E-05	0.1	9.0E-06	0.1

Impact categories with grey background represent 80% of the sum of normalised impacts. For each plasticiser, the first column shows the PB-normalised result (adimensional), while the second column shows its share over the sum of all impact categories

2.3.4.6 Conclusions for step 4

Based on the LCA results, none of the alternative performed sufficiently 20% better than the reference used for all the impact categories, with the exception of ESBO for resources use fossil due to the fact that is a bio-based plasticiser. Therefore we could not identify any alternative plasticiser to DEHP that would be present lower environmental impacts in the different categories. However, there are impact categories in which some alternatives perform better such as DINCH and ESBO in photochemical ozone formation (score 2) or DINCH, DEHT and ESBO in particulate matter (score 2).

Nonetheless, the LCA present detailed results that can support the chemical producer to improve the environmental performance as it allows to identify what are the most impactful impact category, life cycle stage, and process to be improved. This information can be used in the re-design of a chemical/material production process for example.

A relevant challenges to point out is the complexity in performing a cradle to grave LCA of a chemical/material, in this specific case, a plasticiser. To be able to conduct the study, a company performing the assessment along the supply-chain should be able to engage with its supplier and customers in order to follow the production of a chemical and its use. However, each step in the supply chain has specific challenges in the data collection. The plasticiser manufacturer on one side, might not know exactly how their product is used in the formulation and in which market is actually used. Formulators on the other side know how the plasticiser is used in their market, but they do not have information on how the plasticiser or its precursors are made by different suppliers.

This problem can be addressed if the information regarding environmental performance is shared across the supply-chain.

Finally, information regarding the use phase and the end-of-life of the product are needed to have a complete picture of the life cycle. However, this information is strictly related to consumer behaviours, regional waste management practises and legislation, hence they are out of the control of the companies in the value-chain of the product. To address this issue, it may be useful to develop a set of waste treatment scenario and datasets to be used by companies in order to check the environmental profile under different assumptions.

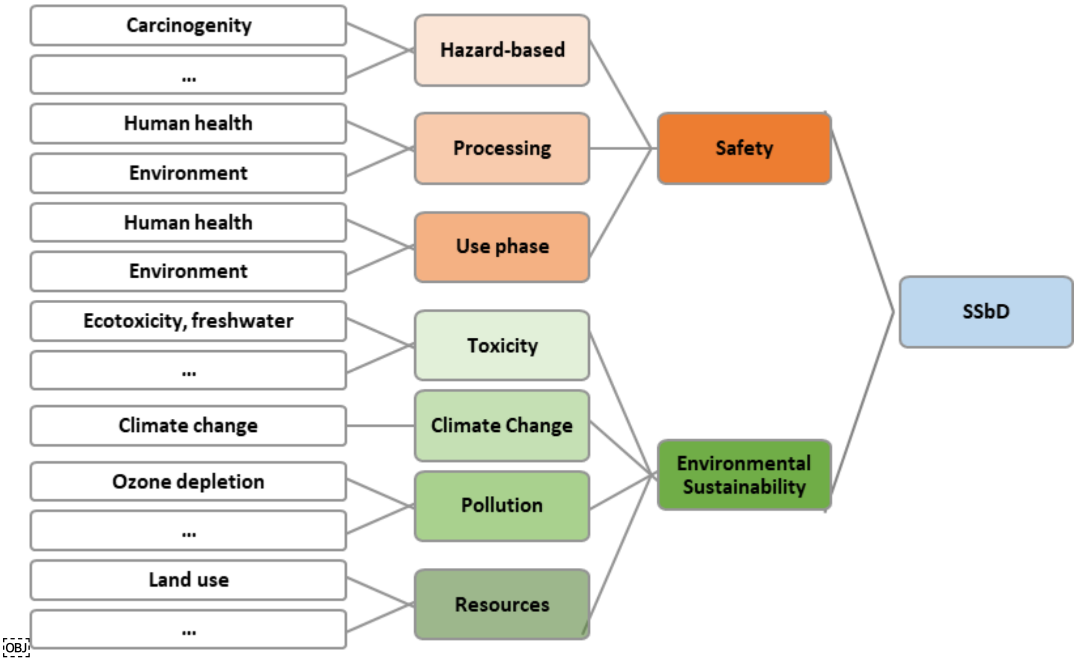
2.3.5 Overall assessment of SSbD performance

In this section, an overview of the assessment performed in each step is presented. It is important to note that this scoring system is not definitive, and it is used only to illustrate options for scoring in order to facilitate communication and decision-making.

A SSbD score is obtained by aggregating the scores for safety and environmental sustainability which in turn are obtained with the aggregation of scores for each step (in the safety case) or of each impact group (for the environmental sustainability, as illustrated in Figure 19.

Multi Criteria Decision Analysis (MCDA) methods can be used to perform this aggregation and several options exist. In this case, the method used to aggregate the scores considers additional minimum requirements. It degrades the SSbD level from 3 to 2 if any of the scores is 0. As a consequence, a minimum level of 1 on all the scores is required to reach SSbD level 3.[29] This method disallows complete compensation among the scores; namely, this disallows granting the top SSbD score to a chemical that includes any element of high concern, no matter how good it is in the other aspects.

Figure 19. Aggregation of safety and environmental aspects as a hierarchy



2.3.5.1 Step 1 Hazard Assessment

Step 1 indicates the 'hazard level' in which the chemical/material falls when applying the SSbD criteria for the hazard properties. The level is given on a scale ranging from Level 0 to Level 3. The level is defined by conditions related with hazard properties without involving any aggregation, and therefore no MCDA methods are required in this step. The scoring for step 3 is presented in Table 53.

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[29] This could become more demanding, e.g, requiring a minimum level of 1 to reach level 2 as well.

Table 53. SSbD scoring for Step 1

Plasticiser	SSbD Step 1
DEHP	0
ATBC	3
DEHA	3
DEHT	3
DINCH	3
ESBO	3

2.3.5.2 Step 2 Human health and safety aspects in production and processing phase

Step 2 indicates if the production and processing of the plasticisers poses any risk to human health of the workers. The level is given on a scale ranging from Level 0 to Level 3. The level depends on whether the total Risk Characterization Ratio (RCR) is less than 1 (level 3) and whether the number of individual contributing scenarios RCRs is greater than 1 is zero (granting Level 2), one (Level 1), or more than one (Level 0).

Each stage (manufacturing of the plasticiser, formulation of the plastisol and production of the gasket) will have a number of Contributing Scenarios (REACH's PROCs - Process categories concerning human health and ERC- Environmental Release Categories), each one scored 0-3. Therefore, aggregation methods need to be applied within this step.

Below, Table 54 shows the overall results for the step 2 with the aggregation method described above. However, the situation would be different if any PROC or ERC presented Level 0 (more than one Contributing Scenarios with RCR>1), in which case the resulting SSbD level for Step 3 would be capped to Level 2.

Table 54. Aggregated score for Step 2

	Manufacture		**Formulation**		**Plastic article**		**Average**	**SSbD level**
	HH	**ENV**	**HH**	**ENV**	**HH**	**ENV**		**Step 2**
DEHP	3	3	3	3	3	3	3	3
ATBC	3	3	2	3	2	3	2.7	3
DEHA	3	3	3	3	3	3	3	3
DEHT	3	3	3	3	3	3	3	3
DINCH	3	3	3	3	3	3	3	3
ESBO	3	3	3	3	3	3	3	3

2.3.5.3 Step 3 Human health and environmental aspects in the final application

Step 3 concerns the final consumers' exposure by ingestion to the plasticisers through the food. The level is given on a scale ranging from Level 0 to Level 3. In this case study, the level depends on whether the total Risk Characterization Ratio (RCR): Level 3 corresponds to an RCR less than 0.5, Level 2 corresponds to an RCR in the range of 0.75-1, Level 1 corresponds to an RCR in the range of 1-1.5, and Level 0 corresponds to an RCR above 1.5.

No MCDA methods are required in this step. The preliminary results obtained show the level depends on the food system in which the plasticiser is applied (Table 11). Table 55 shows the results obtained.

Table 55. SSbD scoring for Step 3

	Chocolate	**Clear drinks**	**Dry pasta**	**Milk**	**Olive oil**	**Orange juice**	**Tomato sauce**	**Yogurt**
DEHP	2	0	0	2	3	1	0	2
ATBC	3	3	3	3	3	3	3	3
DEHA	3	3	3	3	3	3	3	3
DEHT	3	3	3	3	3	3	3	3
DINCH	3	3	3	3	3	3	3	3
ESBO	3	3	3	3	3	3	3	3

2.3.5.4 Step 4 Environmental Sustainability

Step 4 assesses the environmental impacts of the plasticiser along its entire life cycle, using the Environmental Footprint method. For each one of the 16 impact categories encompassed by this method, the life cycle impacts are computed. In turn, these are transformed into 16 dimensionless values (scores on scale 0-3) by comparing these impacts with some reference values: Level 3 corresponds to a 20% reduction (or better), Level 2 corresponds to a reduction between 5% and 20%, Level 1 corresponds to being in-between a reduction of 5% and an increase of 10%, and Level 0 corresponds to an increase of 10% or more in relation to the reference. The reference considered in the case study was one of the plasticisers, DEHP, which always obtains a Level 1 rating according to the previous boundaries. **These boundaries separating the successive levels are not definitive yet** and are presented for illustrative purpose. The results are presented in Table 56.

Table 56. Results of scoring for environmental sustainability

	Percentage change						**Scoring**					
Impact category	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Human toxicity, cancer	0%	18%	67%	-1%	-14%	37%	1	0	0	1	2	0
Human toxixcity, non cancer	0%	31%	9%	0%	-11%	-2%	1	0	1	1	2	1
Ecotoxicity, freshwater	0%	22%	4%	-1%	-6%	6%	1	0	1	1	2	1
Climate change	0%	8%	36%	-1%	4%	32%	1	1	0	1	1	0
Ozone depletion	0%	7%	7%	0%	-12%	-11%	1	1	1	1	2	2
Particulate matter	0%	23%	21%	-10%	-14%	-10%	1	0	0	2	2	2
Ionizing radiation, Human Health	0%	9%	1%	0%	6%	-11%	1	1	1	1	1	2
Photochemical ozone formation, human health	0%	14%	9%	-8%	-8%	-9%	1	0	1	2	2	2
Acidification	0%	28%	14%	-4%	-7%	-10%	1	0	0	1	2	2
Eutrophication, terrestrial	0%	40%	16%	-2%	-5%	3%	1	0	0	1	1	1
Eutrophication, freshwater	0%	17%	7%	-1%	-11%	1%	1	0	1	1	2	1
Eutrophication, marine	0%	41%	10%	-3%	-6%	146%	1	0	0	1	2	0
Water use	0%	49%	2%	-1%	202%	0%	1	0	1	1	0	1
Land use	0%	665%	8%	-1%	-6%	327%	1	0	1	1	2	0
Resource use, fossil	0%	2%	6%	-2%	2%	-31%	1	1	1	1	1	3
Resource use, minerals and metals	0%	40%	11%	3%	-13%	12%	1	0	0	1	2	0

Caldeira et al. (2022b) proposes an aggregation to determine a Level for each impact category group:

- **Toxicity (ES1),** aggregating Human toxicity - cancer, Human toxicity - non cancer, and Ecotoxicity - freshwater
- **Climate change (ES2),** a group on its own, not requiring aggregation
- **Pollution (ES3**), aggregating Ozone depletion, Particulate matter, Ionizing radiation - Human Health, Photochemical ozone formation - human health, Acidification, Eutrophication - terrestrial, Eutrophication - freshwater, and Eutrophication - marine
- **Resources (ES4),** aggregating Water use, Land use, Resource use - fossil, and Resource use - minerals and metals.

An important aspect to note is that **some of the impacts rated as Level 0 are much worse than the reference**. This provides an additional argument to the method described above to avoid compensation. Results are presented in Table 57.

Optionally, the averages could be weighted to grant more weight to ES1, then ES2, etc., following the hierarchy suggested by the JRC draft. By placing more weight on ES1 and ES2 and less weight on ES3 and ES4, the SSbD rating of ESBO could decrease to 0.

Table 57. Scoring obtained for each impact group

	Toxicity		**Climate Change**	**Pollution**		**Resources**		**SSbD Step 4**	
	Average	**Level**	**Level**	**Average**	**Level**	**Average**	**Level**	**Average**	**Level**
DEHP	1.00	1	1	1.00	1	1.00	1	1.00	1
ATBC	0.00	0	1	0.25	0	0.25	0	0.25	0
DEHA	0.67	1	0	0.50	0	0.75	1	0.50	0
DEHT	1.00	1	1	1.25	1	1.00	1	1.00	1
DINCH	2.00	2	1	1.75	2	1.25	1	1.50	2
ESBO	0.67	1	0	1.50	2	1.00	1	1.00	1

2.3.5.5 Safety, Environmental Sustainability, and SSbD score

MCDA can also be used to aggregate Steps 1-3 into a Hazard and Safety level, and to aggregate the latter with the Score from Step 4, according to the structure in Figure 19. To prevent compensation of lower scores a minimum level of 1 in Steps 1-3 could be a condition to reach level 2 and a minimum level of 2 could be a condition to reach level 3. An even less compensatory logic could be followed at this stage, considering the level for the Hazard and Safety would be the minimum level among steps 1-3, as presented in Table 58. This logic is fully consistent with the idea expressed in the framework that chemicals failing to pass any of these criteria would not be allowed to be considered SSbD (Caldeira et al. 2022b).

Table 58. Scores for step 3

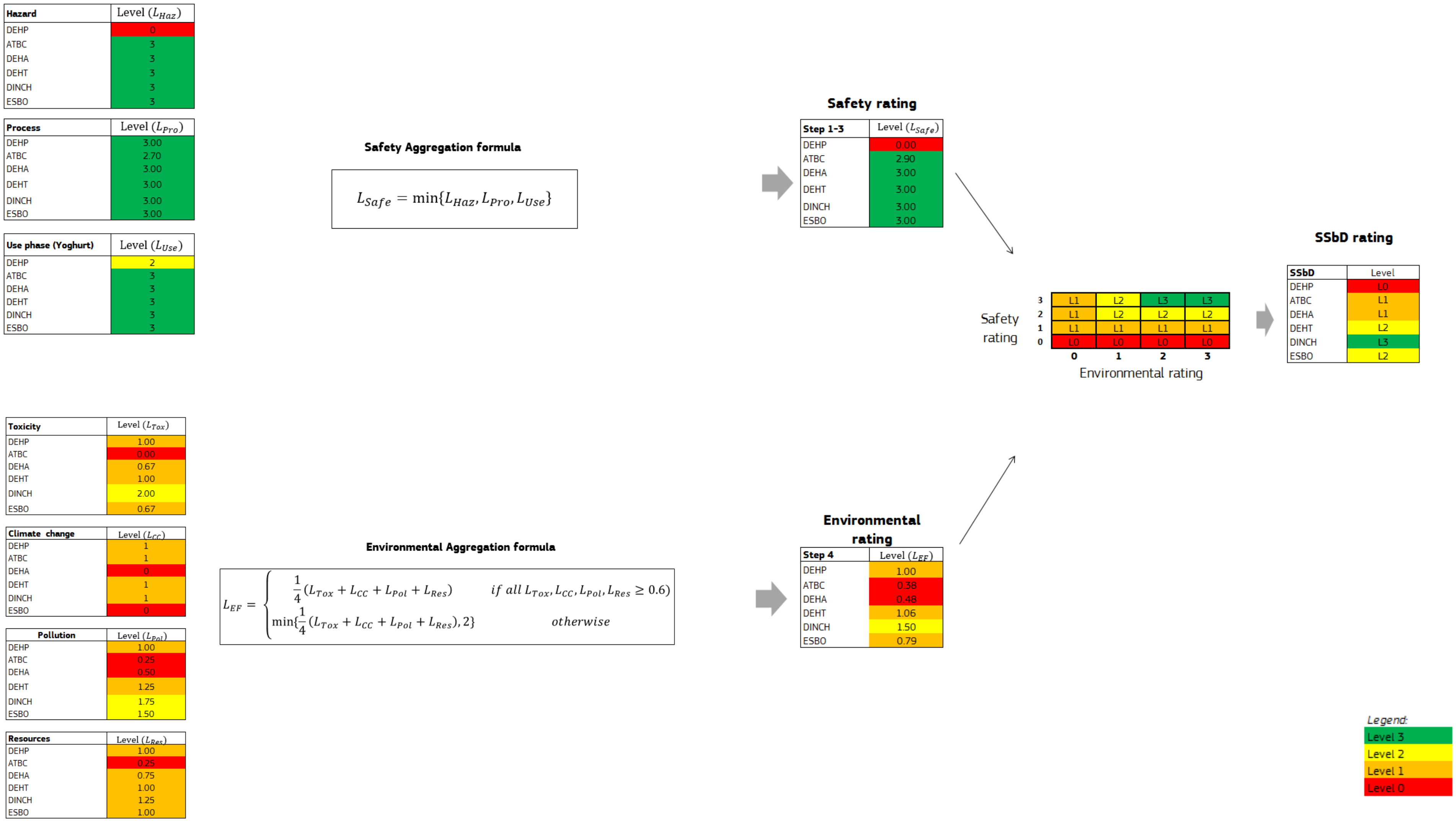
	Hazard Level	Processing Average	Level	Use phase Level	Worst level
DEHP	0	3	3	2	0
ATBC	3	2.7	3	3	3
DEHA	3	3	3	3	3
DEHT	3	3	3	3	3
DINCH	3	3	3	3	3
ESBO	3	3	3	3	3

Finally, the aggregation of Hazard Safety level and Step 4 (Environmental footprint) could follow a simple aggregation table, as exemplified in Table 59 with a two-way aggregation considering homogeneous rating scales (4 levels). The Safety dimension is prioritized: a rating L in Safety and L-1 in Environment is never worse than the contrary. The resulting tree, for the Yoghurt case, would then be the one depicted in Figure 20.

Table 59. Two-way aggregation table. Safety dimension is prioritized: a rating L in Safety and L-1 in Environment is never worse than the contrary

		Environmental rating			
		0	**1**	**2**	**3**
Safety rating	**3**	L1	L2	L3	L3
	2	L1	L2	L2	L2
	1	L1	L1	L1	L1
	0	L0	L0	L0	L0

Figure 20. Levels hierarchy illustrated with the case of yoghurt in step 3.



Hazard	Level (L_{Haz})
DEHP	0
ATBC	3
DEHA	3
DEHT	3
DINCH	3
ESBO	3

Process	Level (L_{Pro})
DEHP	3.00
ATBC	2.70
DEHA	3.00
DEHT	3.00
DINCH	3.00
ESBO	3.00

Use phase (Yoghurt)	Level (L_{Use})
DEHP	2
ATBC	3
DEHA	3
DEHT	3
DINCH	3
ESBO	3

Safety Aggregation formula

$$L_{Safe} = \min\{L_{Haz}, L_{Pro}, L_{Use}\}$$

Safety rating

Step 1-3	Level (L_{Safe})
DEHP	0.00
ATBC	2.90
DEHA	3.00
DEHT	3.00
DINCH	3.00
ESBO	3.00

Toxicity	Level (L_{Tox})
DEHP	1.00
ATBC	0.00
DEHA	0.67
DEHT	1.00
DINCH	2.00
ESBO	0.67

Climate change	Level (L_{CC})
DEHP	1
ATBC	1
DEHA	0
DEHT	1
DINCH	1
ESBO	0

Pollution	Level (L_{Pol})
DEHP	1.00
ATBC	0.25
DEHA	0.50
DEHT	1.25
DINCH	1.75
ESBO	1.50

Resources	Level (L_{Res})
DEHP	1.00
ATBC	0.25
DEHA	0.75
DEHT	1.00
DINCH	1.25
ESBO	1.00

Environmental Aggregation formula

$$L_{EF} = \begin{cases} \frac{1}{4}(L_{Tox} + L_{CC} + L_{Pol} + L_{Res}) & if\ all\ L_{Tox}, L_{CC}, L_{Pol}, L_{Res} \geq 0.6) \\ \min\{\frac{1}{4}(L_{Tox} + L_{CC} + L_{Pol} + L_{Res}), 2\} & otherwise \end{cases}$$

Environmental rating

Step 4	Level (L_{EF})
DEHP	1.00
ATBC	0.38
DEHA	0.48
DEHT	1.06
DINCH	1.50
ESBO	0.79

Safety rating				
3	L1	L2	L3	L3
2	L1	L2	L2	L2
1	L1	L1	L1	L1
0	L0	L0	L0	L0
	0	**1**	**2**	**3**

Environmental rating

SSbD rating

SSbD	Level
DEHP	L0
ATBC	L1
DEHA	L1
DEHT	L2
DINCH	L3
ESBO	L2

Legend:
🟩 Level 3
🟨 Level 2
🟧 Level 1
🟥 Level 0

It should be noted that the resulting SSbD level is a single piece of information that summarizes, but also hides, all the information that was considered in the assessments. Therefore, it would be recommendable to not communicate this rating alone. At a minimum, the next level in the hierarchy would also be communicated. Since this might still omit potential elements for concern, and in these cases additional information that allows to point out any concern could be added as a footnote as illustrated in Table 60.

Table 60. Levels for the safety and environmental sustainability

Chemical	Hazard	Processing	Use phase	**Safety**	Toxicity	Climate change	Pollution	Resources	**Environmental Sustainability(*)**	**SSbD Level**
DEHP	0	3.00	2	**0.00**	1.00	1	1.00	1.00	**1.00**	**0**
ATBC	3	2.70	3	**2.90**	0.00	1	0.25	0.25	**0.38**	**1**
DEHA	3	3.00	3	**3.00**	0.67	0	0.50	0.75	**0.48**	**1**
DEHT	3	3.00	3	**3.00**	1.00	1	1.25	1.00	**1.06**	**2**
DINCH	3	3.00	3	**3.00**	2.00	1	1.75	1.25	**1.50**	**3**
ESBO	3	3.00	3	**3.00**	0.67	0	1.50	1.00	**0.79**	**2 (1)**

(*) Relatively to the impacts of DEHP, considered as a reference for the assessment

Elements of concern to be noticed:

(1) ESBO: Level 0 in Climate Change represents a 32% increase in emissions, Level 1 in Toxicity includes a 37% increase in Human toxicity – cancer emissions, Level 1 in Resources includes a 146% increase in Marine eutrophication emissions, and level 1 in Resources includes a 327% increase in Land use (all increases when compared to the DEHP reference).

2.4 Exploratory assessment of socio-economic sustainability

The framework proposed by Caldeira et al. (2022b) suggests an exploratory approach for the assessment of socio-economic sustainability, which was explored and is presented in this section. The socio-economic impacts associated to alternative gaskets were assessed, using three production systems based on potential supply chains. The methodology used to perform the analysis is based on a simplified Social Life Cycle Assessment (S-LCA) using a reference scale assessment method, which can be enriched when company data are available (Harmens Goedkoop, 2021; UNEP, 2020; Goedkoop et al. 2020). In addition, considerations on how to address economic aspects related to the materials criticality are presented as well.

The aim of this part is to investigate if the current availability of methods and data can support the development of socio-economic criteria for the SSbD of chemicals and materials and which are the main challenges for their implementation.

The chapter is structured as follows: the first part describes how the simplified S-LCA was applied to different gaskets in a food contact application, manufactured using alternative plasticisers. The second part presents some ideas on how economic considerations on materials criticality could complement the analysis.

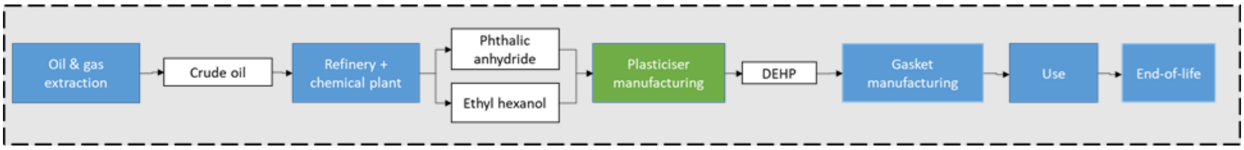
2.4.1 Definition of product systems

In the social assessment, the definition of a product system consists in the collection of interconnected processes in the life cycle of a product. For each process, a geographical location and a sector should be identified, in order to represent a likely supply chain. When developing a simplified social assessment like those proposed here, quantitative information on the amounts of inputs flowing in the supply chain is not needed, but country-specific sector involved in the life cycle of the product under consideration is required.

In the case of plasticisers used in gaskets, when considering the alternatives analysed in the environmental analysis, chemicals based on Phthalic anhydride and Ethyl Hexanol show no differences in terms of countries and sectors involved in the supply chain. Therefore, a product system can be developed which starts from the extraction of fossil fuels and that can represent the following alternatives (Figure 21.):

- Di-(2-ethyl hexyl) Phthalate – DEHP;
- Di(2-ethyl hexyl) Terephthalate – DEHT;
- Di-isononyl cyclohexanoate – DINCH;
- Di(2-ethyl hexyl) Adipate – DEHA).

Figure 21. Product system for the social assessment alternative gaskets based on DEHP, DEHT, DINCH and DEHA



Based on the above product system, alternative supply chains can be modelled, based on the selection of likely country-specific sectors for each phase of the supply chain. Using statistics on production and trade (OEC, 2022), four possible supply chains are listed for illustrative purposes, reflecting various locations in each phase of the supply chain (Table 61)[30].

Table 61. Locations for each phase of a fossil fuel-based gaskets life cycle, for four different alternative supply chains

	Oil and gas extraction	Refinery and chemical plant	Plasticiser manufacturing	Manufacture of gasket	Use	Waste management
S1	Russia	Germany	Germany	Germany	Germany	Germany
S2	UK	Germany	Germany	Germany	Germany	Germany
S3	China	China	Spain	Spain	Spain	Spain
S4	Saudi Arabia	Saudi Arabia	Italy	Italy	Italy	Italy

In the case of the gaskets based on ESBO and ATBC, Figure 22 and Figure 23 show the supply chains for these products and the related tables (Table 61 and 62) indicate potential locations where each phase of the supply chain can operate.

Figure 22. Product system for the social assessment of gaskets based on ESBO plasticiser

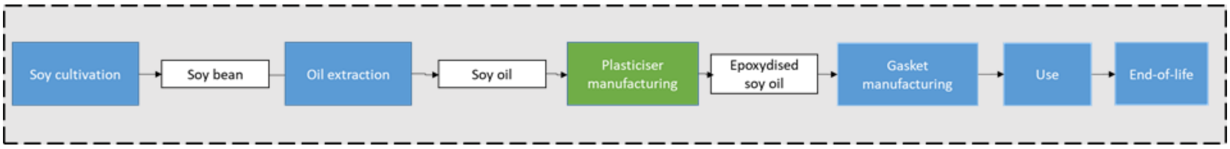
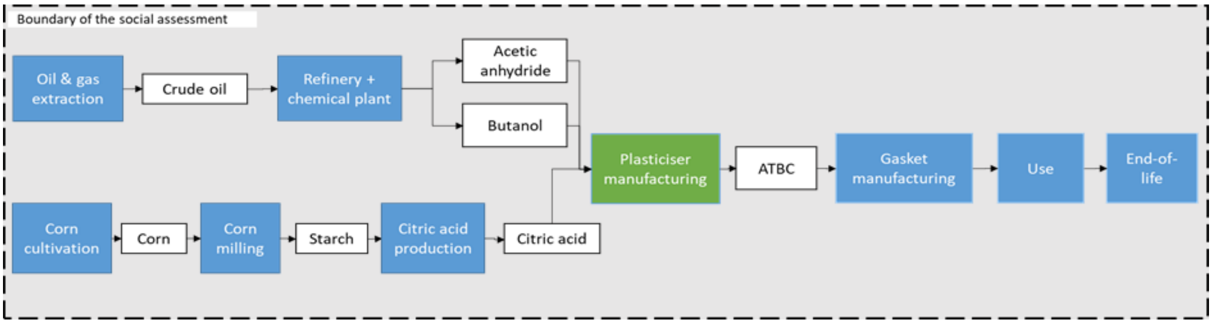


Table 62. Locations for each phase of gasket life cycle based on ESBO

	Soy cultivation	Oil extraction	Plasticiser manufacturing	Manufacture of gasket	Use	Waste management
S5	United States	Germany	Germany	Germany	Germany	Germany

Figure 23. Product system for the social assessment of gaskets based on ATBC plasticiser



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[30] The four systems defined in Table 61 are not representing a specific alternative of plasticiser.

Table 63. Locations for each phase of gasket life cycle based on ATBC plasticiser

	Oil and gas extraction	**Refinery and chemical plant**	**Corn cultivation**	**Corn milling**	**Plasticiser manufacturing**	**Manufacture of gasket**	**Use**	**Waste management**
S6	Libya	Germany	Brazil	Brazil	Germany	Germany	Germany	Germany

2.4.2 Selection of stakeholder categories, impact subcategories and indicators

The selection of relevant categories of stakeholders and impacts subcategories is discussed in Caldeira et al. (2022b) and resulted in the list shown in Table 64. This table also shows the availability of data and their aggregation level, and based on this aspect, the decision of including or not the social category in the assessment. Given that limited data availability do not allow the assessment of impact for local communities, the social category indigenous rights was added in the list. In particular, in the case of local communities impacts the data at country level available in the database used for the assessment is not enough specific to assess this type of impact.

The assessment of these social aspects can be based on primary data (collected on site and/or provided by companies) and on secondary data (from literature or databases). The steps of the supply chain which are assessed using primary data (that there for can be investigated more in depth) constitutes the so-called foreground system, while the background system refers to all the phases of the supply chain that are assessed using secondary data. In this case study, only secondary data were used to assess the selected impact subcategories and rely mainly on the databases PSILCA (Product Social Impact Life Cycle Assessment) and ILOSTAT for the data gathering.

Table 64. List of social aspects selected in Caldeira et al. (2022b)

Stakeholder category	**Social impact subcategory**	**Data availability and source at country/sector level**	**Inclusion in the assessment**
Workers	Child labour	ILOStat (country)	yes
	Fair salary	PSILCA (country-sector)	yes
	Forced labour	PSILCA and Walk Free Foundation (country)	yes
	Health and Safety (not captured in other steps[31])	ILOStat (country-sector)	yes
	Freedom of association and collective bargaining	PSILCA (country)	yes
	Working hours	PSILCA (country-sector)	yes
	Equal opportunities / discrimination	PSILCA (country-sector)	yes
Local community	Community engagement	Not available	no
	Local employment	PSILCA (country)	no, as country level assessment is not enough meaningful for this impact category
	Respect of indigenous rights	PSILCA (country)	yes
Consumers	Responsible communication	Not available	no (due to lack of data)
	Health and safety (not captured in other steps[32])	Not available	no (due to lack of data)

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[31] i.e. fatal and non-fatal accidents at work, presence of sufficient safety measures, DALYs due to indoor and outdoor air and water pollution, Violations of mandatory health and safety standards, Workers affected by natural disasters (cfr. Eisfeldt, 2017).

[32] e.g. Number of consumer complaints; number of defects detected per production batch; presence of management measures to assess consumer health and safety, etc (UNEP, 2021).

The set of indicators used in this study to assess the background system is listed in Table 65. The list is derived from the database PSILCA. PSILCA is based on the combination of a multi-regional input/output database, i.e. Eora (Lenzen et al., 2013), with a database including statistics on the diverse social aspects covered in the indicators. Based on Eora, PSILCA contains an inventory of monetary exchanges for almost 15,000 industry sectors and commodities in 189 countries. Besides, it includes social indicators for each country-specific sectors. Social indicators are structured according to the UNEP's social LCA framework (UNEP, 2020) including five stakeholders' categories and 23 impact subcategories (e.g. child labour, fair salary, etc.). A total of 87 indicators address negative impacts or social risks, apart from the indicator "contribution to economic development" that refers to a positive impact or a social opportunity.

Regarding social data in PSILCA, most sources used in the database are obtained from recognized official statistical agencies, such as International Labour Organization (ILOstat[33]) and from other well-established public or private sources. The PSILCA database also offers a data quality evaluation for each data point, assessed based on its technical and geographical conformance, i.e. if a data point is specific for the sector and the country (and not estimated or extrapolated); for its temporal conformance (i.e. if is up-to date); its completeness and considering the data source reliability. Moreover, a reference scale defining the level of risk for each indicator value is provided by the database.

The social indicators included in PSILCA allow assessing various stakeholder categories, but consumers are not included in the current version of the database and therefore cannot be assessed. Concerning the impact subcategories linked to local communities, "community engagement" is not present in the database, while the subcategory "local employment" is assessed with an indicator on the general level of unemployment in a country, and therefore is not considered meaningful enough to assess the impact on local community. These impact subcategories, therefore, can be assessed only for the foreground system and are left out from this study. "Indigenous rights" is instead an impact subcategory which can be assessed using data at country level (at least in terms of risk that indigenous populations can be affected by a production activity) and was added in the list of social indicators.

The indicators proposed for the background system (Table 65) allows the assessment of the supply chain at country-sector level using secondary data (statistics, estimates and data from literature). This analysis can be complemented and enriched by primary data collected at company level in order to assess the so-called foreground system.

A set of indicators that can be used for the primary data collection at company level, i.e. for the foreground system, is available in Annex 10. While this type of analysis is not performed here, a company can use this list to evaluate the own level of performance/risk and those of direct suppliers. The reference scale suggested in Goedkoop et al. (2020), which refers to company performance and levels of improvement, can be used to assess the performance of the company under investigation.

Table 65. List of indicators to assess the background system. Source: PSILCA database (Eisfeldt, 2017)

Stakeholder category	Social impact subcategories	Indicators for background processes	Unit
Workers	Child labour	Children in employment, male	%
Workers	Child labour	Children in employment, female	%
Workers	Child labour	Children in employment, total	%
Workers	Fair salary	Living wage, per month	USD
Workers	Fair salary	Minimum wage, per month	USD
Workers	Fair salary	Sector average wage, per month	USD
Workers	Forced labour	Trafficking in persons	Tier
Workers	Forced labour	Frequency of forced labour	%
Workers	Forced labour	Goods produced by forced labour	Yes/no
Workers	Health and Safety	Rate of non-fatal accidents at workplace	%
Workers	Health and Safety	DALYs due to indoor and outdoor air and water pollution	DALY rate
Workers	Health and Safety	Rate of fatal accidents at workplace	%
Workers	Health and Safety	Presence of sufficient safety measures	Yes/no
Workers	Health and Safety	Workers affected by natural disasters	%

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[33] https://ilostat.ilo.org/

Stakeholder category	Social impact subcategories	Indicators for background processes	Unit
Workers	Health and Safety	Violations of mandatory health and safety standards	ratio
Workers	Freedom of association and collective bargaining	Trade union density	%
Workers	Freedom of association and collective bargaining	Right to strike	Point scale
Workers	Freedom of association and collective bargaining	Right to association	Point scale
Workers	Freedom of association and collective bargaining	Right of collective bargaining	Point scale
Workers	Working hours	Weekly hours of work per employee	hours
Workers	Equal opportunities / discrimination	Women in the sectoral labour force	ratio
Workers	Equal opportunities / discrimination	Gender wage gap	%
Local community	Respect of indigenous rights	Presence of indigenous populations	Yes/no
Local community	Respect of indigenous rights	Indigenous people rights protection index	Point scale

2.4.3 Social inventory and risk assessment

The compilation of the social inventory consisted in retrieving social data and risk values for each indicator, each step of the supply chain, in the six systems under considerations. PSILCA and ILOStat are the main data sources used for this assessment. The reference scales used to assess the risk level for each indicator are available in the Annex 10. They provide quantitative values for each indicator corresponding to the various risk levels. However, when evaluating the social performance at company level, it is also possible to set qualitative indicators and assess the performance of a company with a qualitative reference scale as suggested by Goedkoop (2020). For instance, in the case of occupational health and safety, a performance indicator that can be used to assess the company performance is “presence of a formal policy concerning health and safety” and the reference scale can assess the social performance in qualitative terms (e.g. best in class – generally acceptable situation – unacceptable situation, etc.) and attributing scores that reflect the social performance.

Table 66 shows the results of the assessment, in terms of risk levels for each product system and the impact subcategories under investigation.

Table to Table 72 provide the disaggregated results for each product systems.

None of the system presents very high risk in any of the impact subcategories. Hotspots can be identified in the subcategory “working hours” and “fair salary” (system 4) and in “indigenous rights” (system 5). The high risk on indigenous rights in the system 5 is due to cultivation of soybean in the United States (Table 71). In the case of fair salary and working hours, instead, high risks are linked to the manufacturing sector in Italy.

Looking at the disaggregated results, additional social hotspots (i.e. values equal or minor than 1, indicating high to very high risk) can be observed, e.g.:

- Risk of forced labour and working hours in the Russian extractive sector (system 1, Table 66)
- Child labour in the Chinese extractive sector (system 3, Table 69)
- Freedom of association and collective bargaining in the extractive sector in Saudi Arabia (system 4, Table 70)
- Respect of indigenous rights linked to the EU soybean cultivation (system 5, Table 71)
- Forced labour and Freedom of association and collective bargaining and forced labour in the extractive sector in Libya (system 6, Table 72).

Table 66. Overall risk level results for each product system under investigation*

Social category	System 1	System 2	System 3	System 4	System 5 (ESBO)	System 6 (ATBC)
Child labour	4	4	2	3	4	3
Fair salary	3	3	2	2	2	2
Forced labour	3	3	2	3	3	3
Health and Safety	3	3	2	4	3	3
Freedom of association and c. bargaining	3	3	2	2	3	3
Working hours	2	2	3	1	2	3
Equal opportunities / discrimination	3	2	3	2	2	2
Indigenous rights	2	2	3	n.a.	1	3

* Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available

Table 67. Disaggregated risk level results for product system 1. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 1	Oil and gas extraction – RU	Refinery and chemical plant – DE	Plasticiser manufacturing – DE	Manufacture of gasket – DE	Waste management – DE
Child labour	1.67	4.00	4.00	4.00	4.00
Fair salary	2.00	2.67	2.67	2.67	2.67
Forced labour	1.00	3.00	3.00	3.00	3.00
Health and Safety	4.00	3.33	3.33	3.33	3.33
Freedom of association and collective bargaining	3.25	3.00	3.00	3.00	1.50
Working hours	1.00	2.00	2.00	2.00	2.00
Equal opportunities / discrimination	4.00	2.33	2.33	2.33	2.33
Respect of indigenous rights	2.00	n.a.	n.a.	n.a.	n.a.

* Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available. Country codes: RU: Russian Federation; DE: Germany

Table 68. Disaggregated risk level results for product system 2. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 2	Oil and gas extraction – UK	Refinery and chemical plant – DE	Plasticiser manufacturing – DE	Manufacture of gasket – DE	Waste management – DE
Child labour	4.00	4.00	4.00	4.00	4.00
Fair salary	3.00	2.67	2.67	2.67	2.67
Forced labour	3.00	3.00	3.00	3.00	3.00
Health and Safety	3.80	3.33	3.33	3.33	3.33
Freedom of association and collective bargaining	3.25	3.00	3.00	3.00	1.50
Working hours	3.00	2.00	2.00	2.00	2.00
Equal opportunities / discrimination	2.00	2.33	2.33	2.33	2.33
Respect of indigenous rights	2.00	n.a.	n.a.	n.a.	n.a.

* Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available. Country codes: UK: United Kingdom; DE: Germany

Table 69. Disaggregated risk level results for product system 3. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 3	Oil and gas extraction – CN	Refinery and chemical plant – CN	Plasticiser manufacturing – ES	Manufacture of gasket – ES	Waste management – ES
Child labour	1.00	2.33	3.00	3.00	3.00

System 3	Oil and gas extraction - CN	Refinery and chemical plant – CN	Plasticiser manufacturing – ES	Manufacture of gasket - ES	Waste management - ES
Fair salary	2.67	2.67	2.33	2.33	2.33
Forced labour	1.50	1.50	3.00	3.00	3.00
Health and Safety	1.33	1.33	3.00	3.00	3.00
Freedom of association and collective bargaining	1.50	1.50	3.00	3.00	3.00
Working hours	2.00	2.00	3.00	3.00	3.00
Equal opportunities / discrimination	4.00	4.00	1.50	1.50	1.50
Respect of indigenous rights	2.00	2.00	3.00	3.00	3.00

Table 70. Disaggregated risk level results for product system 4. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 4	Oil and gas extraction – SA	Refinery and chemical plant – SA	Plasticiser manufacturing – IT	Manufacture of gasket - IT	Waste management - IT
Child labour	2.00	1.67	3.00	3.00	3.00
Fair salary	2.33	2.33	1.67	1.67	1.67
Forced labour	2.50	2.50	3.00	3.00	3.00
Health and Safety	4.00**	4.00**	3.50	3.80	3.80
Freedom of association and collective bargaining	1.00	1.00	3.25	3.25	3.25
Working hours	2.00	2.00	1.00	1.00	1.00
Equal opportunities / discrimination	2.00	2.00	2.50	2.50	2.50
Respect of indigenous rights	n.a.	n.a.	n.a.	n.a.	n.a.

Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available. Country codes: SA: Saudi Arabia; IT: Italy. **Data on accidents at work are not available (value based on the other indicators in the social category)

Table 71. Disaggregated risk level results for product system 5. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 5	Soybean cultivation - US	Oil extraction - DE	Plasticiser manufacturing - DE	Manufacture of gasket - DE	Waste management - DE
Child labour	4.00	4.00	4.00	4.00	4.00
Fair salary	2.00	2.67	2.67	2.67	2.67
Forced labour	3.50	3.00	3.00	3.00	3.00
Health and Safety	2.60	3.33	3.33	3.33	3.33
Freedom of association and collective bargaining	2.50	3.00	3.00	3.00	1.50
Working hours	3.00	2.00	2.00	2.00	2.00
Equal opportunities / discrimination	2.00	1.50	1.50	1.50	1.50
Respect of indigenous rights	1.00	n.a.	n.a.	n.a.	n.a.

* Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available. Country codes: US: United States; DE: Germany

Table 72. Disaggregated risk level results for product system 6. Values for each social category corresponds to the average of the risk levels for the corresponding indicators*

System 6	Oil and gas extraction – LY	Corn farming - BR	Corn milling – BR	Refinery - Plasticiser manufacturing - DE	Gasket manufacturing - DE	Waste management - DE
Child labour	1.33	3.33	3.33	4.00	4.00	4.00
Fair salary	2.33	1.33	1.33	2.33	2.33	2.33

Forced labour	0.50	3.00	3.00	3.00	3.00	3.00
Health and Safety	4.00	3.80	3.80	3.00	3.00	3.00
Freedom of association and collective bargaining	1.00	2.50	2.50	3.00	3.00	3.00
Working hours	2.00	3.00	3.00	3.00	3.00	3.00
Equal opportunities / discrimination	4.00	3.00	3.00	1.50	1.50	1.50
Respect of indigenous rights	2.00	4.00	4.00	n.a.	n.a.	n.a.

* Colour code: red: very high risk; orange: high risk; yellow: medium risk; green: low risk; blue: very low risk; grey: data not available. Country codes: LY: Libya; BR: Brazil; DE: Germany.

The case study applied a simplified life cycle social assessment methodology allowing for the detection of social hotspots in the supply chain of alternative gaskets. The use of highly aggregated data (country-sector) does not allow for a detailed analysis of the impacts, but instead only potential risk and hotspots should be discussed.

Uncertainty in the results can derive from various sources, for instance estimates that are used for aspects related to illegal work (child labour and forced labour) are subject to high uncertainty and are not specific for the various sectors, as only country (or regional) estimates are available. Data on accident at work can be affected by quality of the reporting system, which vary from a country to another.

In general, the quality of the analysis may be enhanced if company-based data are used concerning:

- The company performance on specific social indicators (which are eventually used also for sustainability reporting, therefore can be considered low hanging fruits)
- Location of suppliers, at least for tier 1 of the supply chain
- Assessment of suppliers based on due diligence processes

2.4.4 Considerations on economic sustainability

Concerning the economic assessment, LCA-based methodologies rely, beside LCC, on the availability of approaches for the monetary valuation of social and environmental externalities, which at the moment is quite limited. Indeed, as highlighted in Amadei et al. (2021), coefficients for the monetary evaluation proposed in literature show significant variability, and therefore this approach was not applied to the case study.

Other economic considerations mentioned in the SSbD framework (Caldeira et al., 2022b) refer to the criticality of materials used in supply chains. This aspect relates to the economic risk due to supply disruption or sudden raise in materials' cost, deriving from geo-political dynamics or weak governance of exporting countries. This aspect is briefly described in the section below.

2.4.4.1 Presence of Critical Raw Materials (CRMs) in the supply chain

The Chemical Strategy for Sustainability includes the objective of strengthening the EU's open strategic autonomy for some critical chemicals, which can be raw materials but also intermediates or active pharmaceutical ingredients. Indeed, the limited number of suppliers for some chemicals used in essential societal applications may pose risks, for example to the availability of medicines and to EU's capacity to respond to health crises. While the definition and identification of critical chemicals is still in progress, Critical Raw Materials (CRMs) have been assessed at the EU level since 2011 (EC, 2011b) and their consideration in a supply chain analysis could complement the SSbD framework with considerations on the economic risk of the chemicals under investigation.

CRMs are materials with relatively higher economic importance for the EU economy and higher supply risk, due to the high concentration of supply from countries with weak governance (Table 73). The limited substitutability of these materials can also increase materials' criticality which in turn leads to a risk of supply disruption and can be reflected in higher prices in the market. At a design phase, an analysis of life cycle inventories (used in step 4) can allow detecting the presence of CRMs in the supply chain and eventually support the decision-making process when alternative chemicals are compared. Minimizing the amount of CRM in the supply chain can be considered a risk mitigation strategy at company level (as the CRM might be more expensive or less available in the future) and can contribute to relief the EU demand of these materials, for which EU has a high import dependence. However, market dynamics and discovery of new deposits can rapidly change the criticality status, and indeed the CRM list is updated every three years at the EU level. This might be not compatible with the timing of development of new chemicals and release in the market.

In the case of plasticisers, use of CRMs seems not significant as they do not appear in any inventory used for the environmental assessment of the various alternatives (Annex 7). The use of catalysts (which were not included in the LCA phase) could imply the presence of CRMs, even though minimal amounts are usually consumed and therefore they might be excluded from the inventory by cut-off criteria based on mass.

Table 73. List of Critical Raw Materials for the EU in 2023 (EC, 2023a)

Aluminium/Bauxite	Copper	Light rare earth elements	Silicon metal
Antimony	Feldspar	Magnesium	Strontium
Arsenic	Fluorspar	Manganese	Tantalum
Baryte	Gallium	Natural Graphite	Titanium metal
Beryllium	Germanium	Niobium	Tungsten
Bismuth	Hafnium	Platinum group metals	Vanadium
Boron/Borate	Helium	Phosphate Rock	Nickel
Cobalt	Heavy rare earth elements	Phosphorus	
Coking Coal	Lithium	Scandium	

3 Case studies developed by industry

This section presents a brief description of the other two case studies that were developed by companies. The JRC is grateful for their engagement and constructive attitude. Case study 2 was focused on the flame retardants (halogen-free) in Information and communications technology (ICT) products (section 3.1) and case study 3 in surfactants in textiles (section 3.2). Feedback from companies on the application of the framework is presented in section 3.3. The case studies were presented during the 3rd stakeholders' workshop[34]. The slides presented are available in annex 11.

3.1 Case study 2: Flame retardants (halogen-free) in Information and communications technology (ICT) products

This case study was developed simultaneously by two companies: BASF and Clariant.

Short description of the case study developed by BASF

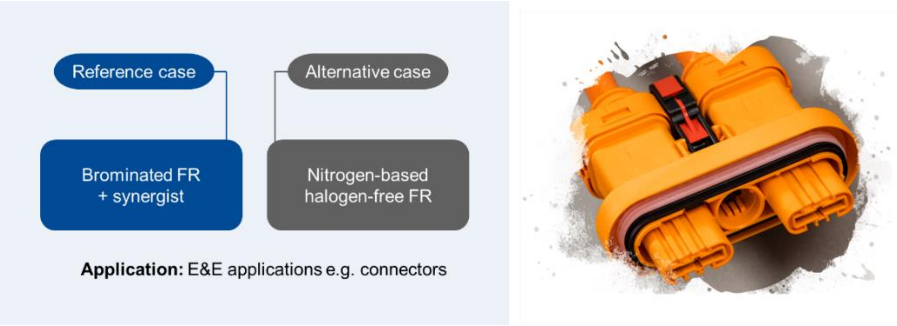
BASF volunteered to participate in the case study to test the SSbD framework developed by JRC. With a strong focus on the flame-retardant substances in the polyamide matrix, BASF evaluates product safety and sustainability along the whole life cycle of the flame retardants and the polymer material itself.

As part of this evaluation the two following role model products were used:

- Polyamide based on PA6, glass fibre and a brominated flame retardant combined with a further synergistic additive
- Polyamide based on PA6, glass fibre and a nitrogen-based halogen-free flame retardant

The final application is the connectors used in ICT products (Figure 22. The system is presented in Figure 23

Figure 24. Illustration of the reference and alternative case and product application (source: BASF presentation at the stakeholder workshop)



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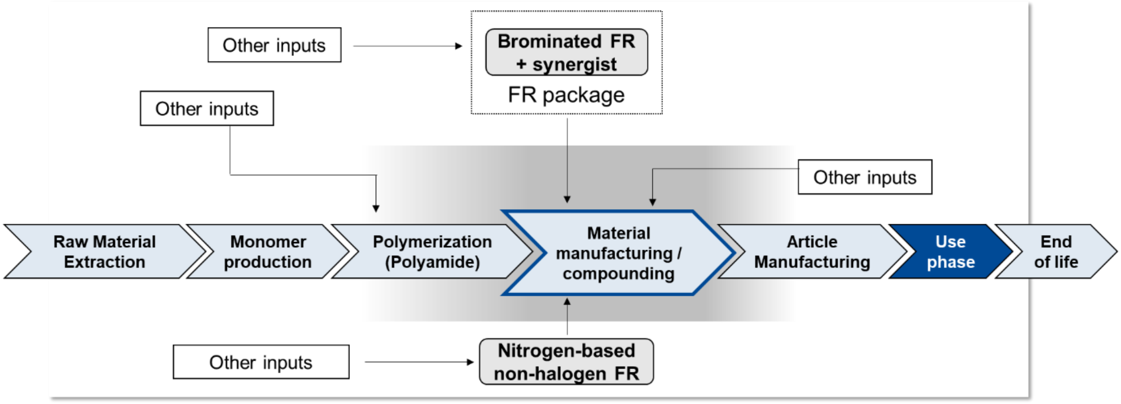
[34] Workshop recordings are available here: day 1 and day 2.

Figure 25. System description of the case study developed by BASF (source: BASF presentation at the stakeholder workshop)



Short description of the case study developed by Clariant

Clariant volunteered to participate in the case study to test the SSbD framework developed by JRC with its flame retardant Exolit® OP 1400.

Exolit OP 1400 is a special flame-retardant grade for polyamides, based on the aluminium salt of diethylphosphinic acid (DEPAL, Alpi) containing a proprietary phosphorus-based synergist:

- Exolit OP 1400 is a non-halogenated flame retardant based on organic phosphinates for reinforced polyamide 6, polyamide 66 and high temperature polyamides. The product achieves its flame-retardant effect through a combined gas phase and condensed phase mode of action.
- The flame retarded polyamide compounds exhibit very good physical and electrical properties. Flame retarded polyamides with Exolit OP 1400 are suitable for applications also in hot and humid environments.

Formulations in polyamides:

- In glass-fibre reinforced polyamide 6 or 6.6, a dosage of about 20 % (by wt.) of Exolit OP 1400 is usually sufficient to obtain the UL 94 V-0 classification for electrical components (at 1.6 mm as well as 0.8 mm and 0.4 mm thickness). In semi-aromatic polyamides the dosage can be reduced to approx. 15%. Subject to the polymer grade, processing conditions and glass-fibre reinforcement the dosage of the flame retardant may vary.

The use case: PA66 GF in ICT equipment:

- A typical application for Exolit in ICT equipment are parts made from glass-fibre reinforced polyamide 66 like USB connectors and sockets on printed circuit boards.

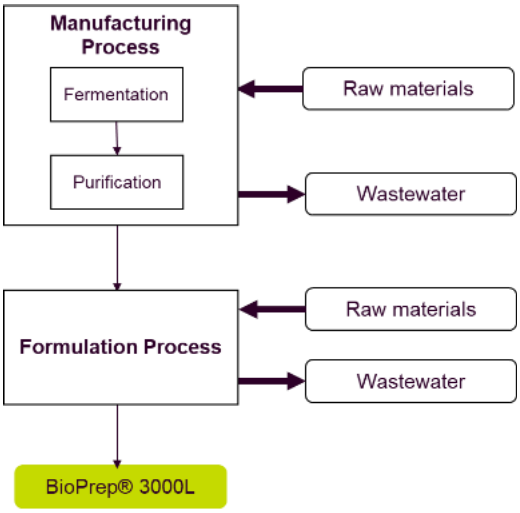
3.2 Case study 3: Surfactants in textiles

Novozymes volunteered to participate in case study 2 for the implementation of the SSbD framework. The case study is about an enzyme - pectate lyase- that is used for scouring of cotton yarns and fabrics in the textile industry reducing energy and chemical consumption in a scouring process[1]. Pectate lyase is formulated with other stabilizers and commercially available as BioPrep® 3000 L.

The system description was provided as follows:

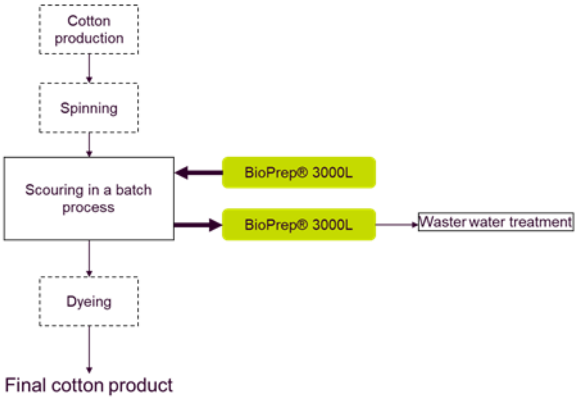
Production: Production takes place Novozymes sites in Denmark. Pectate lyase is an enzyme and manufactured through the fermentation process with a production microorganism. It is further processed in the purification process and formulated with stabilizers. Resulted commercial product is BioPrep® 3000 L.

Figure 26. Description of the manufacturing process (source: Novozymes presentation at the stakeholder workshop)



Use phase: BioPrep® 3000 L is supplied to the textile industry for scouring of cotton. It makes the scouring process simple (one batch process) under milder conditions e.g. moderate temperature and pH and reduce harsh chemicals.

Figure 27. Description of the scouring of cotton in the textile industry (source: Novozymes presentation at the stakeholder workshop)



End-of-life: BioPrep® 3000 L is discharged to wastewater and treated in Sewage Treatment Plant. Due to lack of data the PEF study in step 4 covers simplified end-of-life: wastewater is emitted to nature without treatment

3.3 Feedback from companies

Feedback was collected from the companies developing the case studies, focusing on specific questions:

Question 1. What were your main reasons to participate in the JRC SSbD case study?

BASF

"Most industrial ecosystems depend on chemistry for delivering on the Sustainable Development Goals globally and enabling the Green and Digital transition in Europe. One of the major contributions of the chemical industry to achieve these goals is to innovate towards chemicals that are safe and sustainable.
To evaluate how a company's current portfolio contributes to the purpose of a more sustainable future, BASF developed the Sustainable Solution Steering method in 2012. The objective of Sustainable Solution Steering is

to provide a fully transparent and consistent evaluation of the sustainability performance of BASF's solutions. BASF constantly optimizes this sustainability portfolio assessment method, aiming at a solid and up-dated risks and opportunities evaluation. This has proven to be a valuable source for strategic steering of our portfolio. Hence, applying the JRC SSbD framework may support to further develop the early warning-function of our Sustainable Solution Steering approach.
With the proposed SSbD framework an alternative approach is available, that holistically looks at safety and sustainability along the value chain and may act as a useful supplement for the innovation community developing the solutions for the future. By participating in the SSbD case study it is possible to test and thus conduct a reality check for each step of the framework. This in turn will also help us to check against our currently established portfolio assessment method, but also to develop improvements helping to broadly apply the SSbD framework. A practical and thus successful framework is at the core to support meaningful R&D steering towards the industry transition."

Clariant

"We wanted to understand the SSbD methodology in depth, by applying it to a known product and application

Clariant has been using its own portfolio assessment scheme since 2012 (the Portfolio Value Program). We want to continuously improve and update it. Learnings from SSbD could be included.

We welcome the opportunity to provide qualified feedback to the SSbD framework to make it a practical tool for the chemical industry."

Novozymes

"Enzymes have been used as sustainable solutions in various industries such as textile, paper, animal feed, detergents and food. Novozymes wanted to learn the JRC SSbD framework by joining the case study."

Question 2. What are the main challenges you encountered during the development of the case study?

BASF

"Defining the case study and the system boundaries needs to be very explicit – guidance on how to practically do this may be helpful: The outcome of the assessment could vary, weather the evaluation is conducted on chemicals or the material where the chemical is present.
Identifying and maintain value chain partners, who's input is of great impact for the SSbD assessment (e.g., raw material suppliers): Value chain partners can differ throughout a whole commercial product life cycle, so that initial assumptions may not be applicable in future anymore and the SSbD assessment would not be valid anymore – every assessment is a time-limited snapshot.
Identifying and collecting (generating) the data/information needed for the assessment

- *Step 1: Difficulty to address all endpoint w/o animal tests – here validated screening tests / alternative testing methods need to be agreed to run early-stage assessment for active R&D steering.*
- *Step 2/ Step 3: Accurate data only available for own production steps in the value chain – a limitation of those steps to the in-house production would significantly increase accuracy assessment results. Furthermore, data for the human health and safety assessment in the production/use phase are not available for all substances. Hence, there needs to be a joint understanding about the goal of steps 2 and 3 to prevent usage of industry average values, which in turn will not allow for solid comparison scenarios.*

Step 4: It is extremely time consuming to gather all necessary data, for certain data points only certain assumptions are readily available. Data accuracy is difficult to maintain throughout a product's commercial lifetime, as certain subcategories may vary. For the PEF method there are only limited sets of product category rules available.
Limitations in time and resources: Expertise from different fields required as well as dedicated project management effort is needed to bring together a broad set of expertise to facilitate a single assessment, which will drive time and cost for R&D conducted under this framework."

Clariant

"Defining the case study and the system boundaries: this was not so difficult

Identifying value chain partners: more difficult the farther "away" the value chain partners are, but manageable

Identifying and collecting (generating) the data/information needed for the assessment: a very big hurdle: data needs to be collected from (not only direct) suppliers and customers, some of the data is not readily available, but needs to be generated

Limitations in time and resources: clearly a limiting factor. The PEF assessment was commissioned to a third party at a cost of several 10 k€. Internal resources require expertise from different departments and many person-hours.

Therefore, we strongly advocate to consider a tiered approach with simple screening methods in the early product development stages"

Novozymes

"As we presented during the workshop, we encountered the limitation of a hazard-based cut-off for safe and sustainable chemicals and products. EU has been in the good position for biobased technologies with enzymes. Given our industry long-standing experience in ensuring enzymes' safety, their positive environmental impact and their biological profiles, we believe that enzymes are SSbD ensuring innovation in EU keeping its strong competitive edge.

In Step 2, our company has generated a lot of data in the past 50+ years, so it was relatively straight forward for our case study. On the other hand, a new innovative use would require new exposure assessment – in our case, new actual measurements of enzyme exposures through collaboration with downstream users. A large company can adsorb such resources, but it would be difficult for SMEs to collect all data.

One of the questions raised during the workshop was who is going to make SSbD – is it a manufacturer/importer or downstream users. Thinking about innovations, it can be either or both. Our company is a raw material supplier in B2B business. For us it is difficult to find value chain partners especially when a project is in its early phase

Defining the case study and the system boundaries: in Step 4 we compared two processes (conventional and enzymatic scouring) and since PEF is rather product oriented, we had some doubts when defining the life cycle stages.

Limitations in PEF method (step 4):

- *EF 3.0 impact assessment method lacks factors for direct emissions of pectate lyase (or any other enzyme) to environment, which meant we could not account for impact of enzyme emissions on toxicity;*
- *The underlying toxicity model – USEtox – in current version may not be suitable to derive factors for enzymes, as it does not capture their characteristics;*
- *Lack of a procedure or parameterized dataset for modelling treatment of specific composition of wastewater, which led to simplified end-of-life modeling, not reflecting high degradation rate of enzymes."*

Question 3. What benefits you/your company see after having participated in the SSbD case study?

BASF

"As BASF is highly interested in a commonly applicable SSbD methodology to develop safe and sustainable product portfolios, a test was very helpful to give feedback in the light of applicability for industrial chemical research and innovation. As SSbD is proposed to be a voluntary initiative it is critical to contribute to its applicability to prevent a lack of acceptance in the markets.
The proposed assessment methodology provided various different methods, which BASF is currently evaluating how it could match with the companies Sustainable Solution Steering method."

Clariant

"We will be able to better understand the sustainability profile and impacts for a key product line. This is also useful in responding to increasing number of customer enquiries for PEF data. Sustainability "hotspots" were identified and will be addressed in future developments."

Novozymes

"Overall: We could identify some limitations i.e. the cut-off criteria and issues about USEtox (please see also the below bullet).
(step 4) Better understanding of PEF methodology and its practical application"

Question 4. How do you intend to implement the SSbD (These learnings) in your company/ R&D strategies?

BASF

"BASF constantly revises the sustainability portfolio assessment method (Sustainable Solution Steering method) and some aspects of the framework are of high interest to be evaluated to be adopted within our assessment scheme.
The framework also offers ideas and fruit for thoughts how to integrate quantitative methodologies into an innovation process."

Clariant

"We currently do not foresee the feasibility of doing a full SSbD study on every new development. This can only be done for "flagship" products or major central technology platforms. A comprehensive study as being done now can serve to identify sustainability "hotspots" and aim for specific improvements."

Novozymes

"Our company has implemented 'safety first' policy for R&D strategy, so safety assessment has already been a gate in R&D pipelines in our company. With that said, the learning through case study is that substantiation of sustainability through LCA/PEF is equally critical to safety/risk assessment. Also, EU Transition Pathway describes EU innovation and growth based on amongst others SSbD. The most important learning with the case study is how important it is to assess sustainability through LCA/PEF in an early phase of R&D activities. This learning would be reflected to our company's R&D strategy."

4 Lessons learned and challenges stemming from the application of the SSbD framework

This section illustrates the main issues identified during the application of the SSbD framework stemming from the pilot application to case studies, the workshop, and the related surveys

The 3rd Stakeholder workshop took place the 9th and the 10th of February 2023 to present the case study, and to collect feedback from stakeholders. The recordings are available here: day 1 and day 2. In addition to gathering feedback during the workshop, a dedicated survey was launched to collect feedback to the draft of the present technical report, and to analyse challenges foreseen by stakeholders in order to frame potential actions needed toward the implementation of the SSbD Framework. An agreement among the stakeholders on the **most beneficial application** of the SSbD among stakeholders which is the *"guide the design of new chemicals/materials to be safer and more sustainable"* On the other hand*, stakeholders have different views regarding* **factors that would encourage the implementation** of the SSbD framework. Stakeholders would be mostly encouraged by the *"increase demand for safe and sustainable chemicals/materials directly from customers"* and *"availability of data".* Both imply the necessity of a robust communication between suppliers and customers along the value chain of products.

The **challenges** have been selected as the most important ones include the assessment for chemicals/materials at the early stage of development, the need of specific expertise for each step, and communication, information and data exchange between suppliers. Further details regarding the results of the survey are reported in Annex 12.

An overview of the challenges is presented below. These elements are meant to be the basis for the further development of the SSbD framework. These aspects will be considered for further refinements and should not be considered exhaustive as they will need to be complemented with further input and testing from stakeholders. The multidisciplinary nature of the SSbD framework may allow to assess chemicals and materials more comprehensively but it still presents some challenges.

General elements for the SSbD framework improvement

- Need to clarify the alignment of the SSbD within other initiatives regarding information being requested by them such as Sustainable Finance since this initiative considers criteria for chemicals and chemical products manufacturing (EC, 2023b), or the revision of REACH as for the ambitions of the CSS, that foresee to include environmental footprint information (EC, 2020b).
- Clarification regarding terminology and definitions will be an important aspect to be further assessed and ideally harmonized between the different disciplines underpinning the SSbD (e.g. risk assessment and life cycle assessment) developing an agreed vocabulary to be used in the SSbD context.
- Clarification on the coverage of the steps namely regarding professional uses.
- Clarification of the goal and scope of the SSbD assessment is of high importance. The type of chemical/material, the definition of the production processes, the end of-life stages and the specificity of the final application, for example, influence the approach to the assessment and its output.
- Test of the framework to address, for example: intermediate chemicals/materials with multiple applications, or chemicals/materials at an early stage of development.
- Definition of the solutions to couple the SSbD assessment with the internal design and innovation process.
- Further integration of safety and sustainability dimension implementing life-cycle thinking all along the assessment.
- Ensure the coherence and harmonization of underpinning data in each step of the assessment.
- Availability of data and information remains a challenge for all the steps. Finding a balance between transparency and reproducibility versus confidentiality information is pivotal. Moreover, a key element will be the collaboration across stakeholders for the generation and exchange of data along the supply chains.
- Further exploration of the use of predictive models/tools, including NAMs. The SSbD promotes the use of NAMs for the generation of data to support the assessment. There is already a wide variety of NAMs for the prediction of endpoints for the chemicals hazard assessment. However, there is still a need to

further explore the availability and applicability of these approaches especially in the context of the design and innovation processes. On the other hand, the availability of predictive tools for other assessment steps in the SSbD framework is limited and the possibilities of developing models/tools for these purposes will need to be explored. The standardisation, validation and applicability of these models/tools linked with the quality of the data generated, and how it is integrated in the overall assessment scoring, is another issue that needs further assessed.

- Improvement of data quality and uncertainty assessment is an important factor to be taken into account. Data quality assessment and its associated uncertainty should be included in the process of assessment and subsequent decision making. This is critical also to understand to what extent alternatives that are evaluated using data of different quality can be compared. Ultimately data should be FAIR, i.e. ensuring findability, accessibility, interoperability, and reusability.
- Development of a tiered approach based on Technology Readiness Levels (TRLs) and data availability. In most innovation cases, data (for both hazard and sustainability) is likely to be missing, especially in low TRL. Ideally, the conclusion of each step should not depend on the maturity level of data, rather data requirements and uncertainty levels should be adapted for each step, in function of the TRL level.
- Support the uptake of framework by SMEs, by providing accessible resources for the application of the framework (e.g. databases, sector specific guidance, tools).
- Development of specific skills and training to enable the application of the framework as it requires a wide set of expertise.

Evaluation procedure and scoring system

A procedure to evaluate the chemical/material that supports decision making and also that facilitates communication is important. Specifically, there is the need to improve the informative and discriminating power of the scoring systems to enhance the decision support role of the SSbD during the design and implementation phase of a chemical development, taking into consideration existing trade-offs. Key elements to be addressed include the evaluation procedure, the scoring system (aggregation), the consideration of the data quality and uncertainty, and communication.

- The evaluation procedure is related to the choice of a reference as well as the definition of targets. In this case, the evaluation was based on a reference plasticiser. However, defining such reference might be challenging as one needs to ensure that the reference selected is representative of the chemical/material under assessment.
- The attribution of scores used in this case study was done providing a score from 0 to 3 at each aspect that was assessed and then performing an aggregation among each sustainability dimension and between the safety and sustainability. It used IF-THEN rules for the topmost level aggregation, used the “Min” operator to aggregate Steps 1-3, and a weighed sum plus additional requirements for the remaining aggregation levels. There are, however, challenges on the identification of the best way to build the scoring system and also that trade-offs are unveiled. Other options can be further explored such as aggregating rating levels given as an input to provide an output as a rating level using IF-THEN rules tailoring the aggregation to the level of ambition required (e.g. if a score “0” exists the final score can never be “2”).
- It is important to recall that the communication of results should not consist of only an overall SSbD level and not only intermediate scores should be provided (at least the top ones), but also any elements of concern hidden behind a good overall score (Level 2 or Level 3) should be disclosed.
- An aspect that was not explored is data quality assessment and its use. For this, the purpose of the evaluation needs to be considered. For example, for internal innovation processes, an innovation team might use their best estimates refer to the obtained rating as the “Estimated SSbD rating”, which can be compared with the sought rating as a driver for further innovation and data collection efforts. Another option is to perform quantitative uncertainty analyses that will indicate the “Most likely SSbD rating”, the “Median SSbD rating”, the “Minimum assured SSbD rating”, or even an “SSbD rating 95% confidence interval” to guide innovation decisions. These are aspects to be further investigated.

Step-specific comments

Step 1 Hazard Assessment of the chemical

- The hazard assessment is highly complex, requiring significant amount of data and relying on different resources and expertise. The assessment is not only about the output of the assessment in the form of the CLP classification, but also about the data to conclude on the classification.
- High expertise is needed for all the steps of the hazard assessment:
- Expertise to gather relevant data. In this sense there is the need of tools to search for this kind of data.
- Expertise to assess the data, its quality and reliability, weight and to conclude based on it.
- Expertise to identify data gaps/needs and to build intelligent testing strategies to generate new data.
- Stakeholders consider having cut-off criteria as a potential risk of excluding chemicals/material that can be proven to be safe in a specific application.

Step 2 Human Health and safety aspects in the chemical production and processing

- Company-specific knowledge and data are paramount. The availability of data will influence the result of the assessment from the worst case and unsafe scenario to a more realistic assessment.
- Expertise is needed to:
- Understand the processes in which the chemical/material is involved and build the scenarios
- Identify the appropriate tools and how to use them
- Assess the results

Step 3 Human health and environmental aspects in the final application

- Step 3 assessment shows to be very specific for the product and the product specific regulatory requirements. Therefore, the approach will be different for each case. This adds challenges to identify methodology, data requirements, and available tools for each case. And therefore, the expertise needed will be different each time.
- Communication/information along the supply chain becomes more difficult with the specificity/granularity of this step.

Step 4 Environmental sustainability

- Primary data of the main processes (i.e., gasket manufacturing) are difficult to collect but still available. Primary data of the raw materials are seldom available from suppliers and literature, or datasets are necessary to complete the life cycle inventory. However, this results in a less site-specific modelling.
- The LCA results over the life cycle are product/application specific. If the chemical/material is at the early stage of development, this information is likely to be missing, and methods for prospective LCA, addressing gaps form laboratory to industrial scale, should be applied.
- The SSbD scoring system shows two degrees of detail. The first assigns a score from 0 to 3 for each impact category. The second aggregates those scores into pass/not pass the level. According to the technical report, one level is passed if each impact category belonging to the level scores at least 2. Developing the case study, it is possible to notice that this scoring system can be too demanding and further adjustments could be executed.

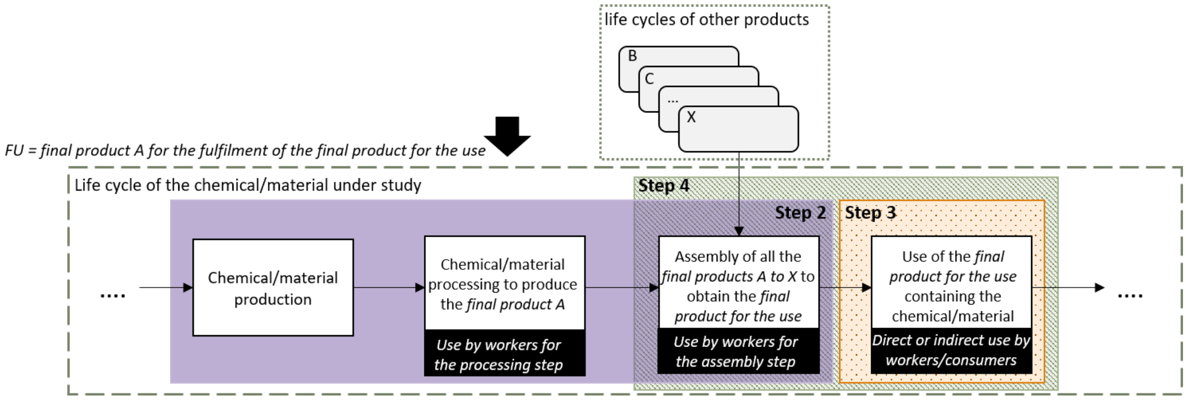
4.1 Further integration of safety and sustainability dimensions

Safety Assessment and Life Cycle Assessment respectively address mostly safety and environmental sustainability aspects. In order to better support SSbD assessment throughout the development of chemicals/materials, the possibility of **integrating the two methodologies** must be further explored. This leads to the necessity of creating an approach that integrates the two aspects to boost the evaluation of the chemical under development. Currently, these two components are applied separately with some similar or apparently overlapping aspects. The integration of the two components is the core of a successful SSbD approach, and it can be particularly beneficial for the design phase where the data are seldom available, the uncertainty is high and expert judgement is needed. It can reduce the data needed and accelerate the assessment at the early stage of a chemical/material development.

The integration of the two methodologies involves a number of challenges, mainly due to **different assessment goals and scopes, underpinning principles, site-specificity, type of assumptions** etc. For instance, the safety assessment is referred to a specific chemical/material by evaluating the actual risk building high specific release scenario(s). It has also an absolute perspective due to the use of background concentrations and thresholds that allows to conclude the safety assessment. Conversely, the LCA considers several chemical/materials linked to a product life cycle, from cradle to grave, and the environmental impact is evaluated by assessing several impact categories. The evaluation is unlike to be local since it considers average landscape conditions, general population and long term impacts. Unlike the safety assessment, the LCA provides relative results without background concentrations and thresholds. This is currently under investigation through the absolute sustainability concept. On the other hand, LCA asses emissions that occur over the entire life cycle.

A critical challenge is the **clarification and harmonization on the respective system boundaries, in particular about the meaning of the *chemical/material use phase*.** So far, regarding the Step 4 (environmental sustainability assessment), a general chemical/material life cycle includes the raw materials extraction, the chemical/material production, the chemical/material processing to produce the final product, the use stage, and end-of-life. In LCA, the use phase is related to the functional unit (FU), implying that all the subsequent steps of the product manufacturing are considered as "use". This partition is quite clear if we aim to assess the impacts of a product put in the market (for example a pair of shoes). However, moving the attention to the chemical/material, the meaning of the use phase becomes unclear. As shown in Figure 28, the *final product A* (for example a pair of soles to fulfil the FU of the pair of shoes) is a component of a *final product for the use* (e.g. a pair of shoes). According to the FU, the assembly step of the *final product A* to obtain the *final product for the use* is part of the use phase. Similarly, if the assessment is focused on the chemical/material (e.g. rubber used for the sole), the use phase would also include the following step *"chemical/material processing to produce the final product A"*. This implies a varying use phase in terms of impacts distribution among the life cycle stages.

Figure 28. How the use phase of the chemical/material is addressed across the steps of the SSbD assessment



Conversely, the use phase of the chemical/material for the safety aspects is split between Step 2 and 3: the workers exposure during the integration processes of the chemical/material in the final product and during the end of its life is analysed in Step 2, and the consumers exposure by the use of the final product containing the chemical/material is assed in Step 3 (Figure 28). However, it is unclear how to consider the exposure of the workers during the use phase of the chemical/material assessed. Hence, there is the need to harmonize the use phase among the two methodologies either according to workers/individuals or to application/use phase.

The different approaches between safety and other sustainability aspects might lead to difficulties in the interpretation of the results and might hamper reliable comparisons among different chemicals/materials by aggregating in different ways the use phase.

4.2 Exploratory assessment of socio-economic sustainability

Regarding the **consideration of socio-economic sustainability aspects**, stakeholders showed contrasting views. In some cases, it was considered very relevant to consider these aspects (with suggestion to be part of the framework) while in other cases the effort needed to perform the assessment and the methodological challenges appear to prevent its applicability.

- As for the safety and environmental assessment, data availability can constraint the applicability of the socio-economic assessment and pose challenges in terms of meaningfulness of the assessment. The access to primary data at company and suppliers level is crucial for enhancing the robustness of the assessment.
- When considering the cost and effort needed to collect this data, synergies between various regulatory requirements should be exploited. For instance, in the case of large companies, the data needed to perform the socio-economic analysis can partially overlap with requirements from the EU legislation like the upcoming due diligence Directive (EC, 2022c) and the corporate sustainability reporting Directive (EU, 2022). Similarly, synergies can be envisaged with the socio-economic analysis required under the REACH procedure on applications for authorisation.
- The selection of a manageable set of social aspects relevant for the chemical sector is also critical in order to derive meaningful insights from the assessment. Finally, further work is needed in order to provide guidance on the interpretation of the results from the socio-economic assessment, in order to better understand how these results can be used to support decision making in the field of chemicals substitution and in the innovation process.

The proposed approaches should be further investigated, taking into account the available methodologies for social foot printing (including the monetization approaches) and their applicability at company level, in order to make them accessible also for SMEs.

5 Conclusions

This report presents the first application of the EC SSbD framework to case studies. Three case studies were selected following a stakeholder consultation and in alignment with relevant EC policies: i) plasticisers (non-phthalate) in food contact materials; ii) flame retardants (halogen-free) in information and communications technology products; and iii) surfactants in textiles processing. Case study i) was developed by the JRC and is presented in detail in this report, including lessons learnt and identified challenges. The other two case studies were conducted by volunteering companies, which provided their feedback on the application of the framework. The case study report was presented in a dedicated SSbD stakeholder workshop (recordings are available) and stakeholders provided feedback on aspects that need further refinements to enhance wide applicability).

A summary of the key aspects stemming from the pilot application to case studies, the workshop and the related surveys[35], are summarised in section 4. These aspects will be considered for further refinements and should not be considered exhaustive. They will need to be complemented with further input and testing from stakeholders. The further development of the framework requires the development of additional case studies to address the different situations for which the framework can be applied (e.g. new chemical being developed, improvement of a production process), having a system perspective and considering alternative approaches to achieve a desired service/function.

A testing phase of the framework is foreseen in the EC Recommendation during which stakeholders can submit results of their case studies. Ideally, these case studies should explore different situations to inform on the applicability of the SSbD framework, especially for what concerns the design and innovation phase. Stakeholders are invited to propose adaptations to the framework or identify the need to develop further tailored guidance. Calls for input by the Commission are foreseen, to collect feedback from stakeholders regarding their involvement on SSbD activities. Their feedback is to be collected through a reporting template to be provided at the announcement of the call[36].

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[35] Further details regarding the results of the survey are reported in Annex 12.

[36] Further information on calls and reporting template will be available at: https://research-and-innovation.ec.europa.eu/news/all-research-and-innovation-news/recommendation-safe-and-sustainable-chemicals-published-2022-12-08_en

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List of abbreviations

AC	Article Category
AESA	Absolute environmental sustainability assessment
ATBC	Acetyl Tributyl Citrate
CAS	Chemical Abstracts Service
CEFIC	European Chemical Industry Council
CEPE	Council of the Paint, Printing Ink and Artists‘ Colours Industry
CF	Characterisation factors
ChemSec	International Chemical Secretariat
Chesar	CHEmical Safety Assessment and Reporting
CLP	Classification, Labelling and Packaging
CMR	Carcinogenic, Mutagenic and Reprotoxic
CRM	Critical raw materials
CS	Contributing scenario
CSS	Chemical Strategy for Sustainability
DEDuCT	Database of Endocrine Disrupting Chemicals and their Toxicity Profiles
DEHA	Di(2-ethyl hexyl) Adipate
DEHP	Di(2-ethyl hexyl) Phthalate
DEHT	Di(2-ethyl hexyl) Terephthalate
DINCH	Di-isononyl Cyclohexanoate
DINP	Di-isononyl Phthalate
DNEL	Derived No-Effect levels for human health
EC	European Commission
ECHA	European Chemicals Agency
ED	Endocrine disruptor
EDslist	Endocrine Disruptor Lists
EF	Environmental Footprint
ELoC	Equivalent level of concern
ENV	Environment
E-PVC	emulsified Polyvinyl chloride
ERC	Environmental Release Category
ESBO	Epoxidized Soybean Oil
EU	European Union
EuPC	European Plastic Converters Association
EUSES	European Union System for the Evaluation of Substances
FAIR	Findable, accessible, interoperable and reusable (data)
FCM	Food Contact Material
FSTP	distribution fractions of the substances in the Sewage Treatment Plant
HH	Human Health

HLC	Henry constant
IATA	Integrated Approaches to Testing and Assessment
ICT	Information and communications technology
ISES	International Society on Exposure Science
IUPAC	International Union for Pure and Applied Chemistry
JRC	Joint Research Centre
Koc	Partitioning coefficients organic matter in soil/water
Kow	partition coefficient octanol-water
LCA	Life Cycle Assessment
LCS	Life cycle stages
LEV	Local Exhaust Ventilation
MCDA	Multi Criteria Decision Analysis
MSC	Member State Committee
MW	Molecular Weight
NAM	New Approach Methodology
NOAEL	No observed adverse effect level
NOEL	No Observed Adverse Effect Levels for human health
NGO	Non-Governmental Organization
OECD	Organisation for Economic Co-operation and Development
OSH	Occupational safety and health
PACT RMOA	Public Activities Coordination Tool-Risk Management Options Analysis
PB	Planetary Boundaries
PBT	Persistent Bioaccumulative and Toxic
PC	Product Category
PEC	Predicted Environmental Concentration
PEF	Product Environmental Footprint
PET	Polyethylene terephthalate
PMT	Persistent Mobile and Toxic
PNECs	Predicted no-effect concentrations
PPE	Personal Protective Equipment
ppm	Parts-per million
PROC	Process category
PVC	Polyvinyl chloride
QSAR	Quantitative Structure Activity Relationships
RCR	Risk Characterization Ratio
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RMM	Risk Management Measures
RoHS	Restriction of Hazardous Substances
RTD	Research and Innovation

SDG	Sustainable Development Goal
SDS	Safety Data Sheet
S-LCA	Social Life Cycle Assessment
SMILES	simplified molecular-input line-entry system
SML	Specific Migration Limit of the chemical
SSbD	Safe and Sustainable by Design
STOT-RE	Specific target organ toxicity - repeated exposure
STOT-SE	Specific target organ toxicity - single exposure
STP	Sewage Treatment Plant
SU	Sector of Use
SVC	Saturated Vapour Concentration
SVHC	Substance of very high concern
TDI	Tolerable Daily Intake
TEDX List	The Endocrine Disruption Exchange list
TF	Technical Function
TRA	Targeted Risk Assessment
TRL	Technology Readiness Level
VP	Vapour pressure
vPvB	very persistent and very bioaccumulative
vPvM	very persistent and very mobile

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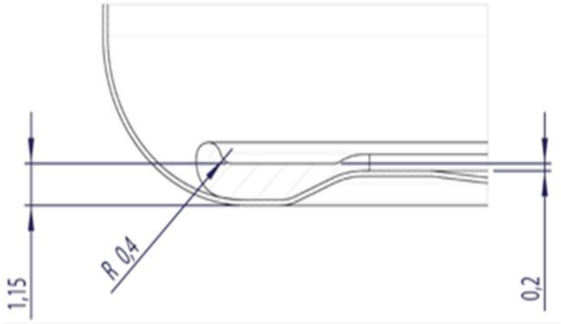
Annexes

Annex 1. Case study – product information

The PVC (i.e., plastisol) sealing gasket/liner used inside the metal caps might be either ring-shaped (e.g. gasket) or disc-shaped (e.g. liner), as mentioned during a consultation with a stakeholder. The ring-shaped gasket has a quite irregular thickness and, as illustrated in Figure A1, it is very thick (1.15 mm) at the edge of the metal cap that corresponds to the part in contact with the glass jar, while it is very thin (0.2 mm) towards the centre of the lid. The disc-shaped gasket has a constant thickness cross the metal lid, which it covers completely. Since the liner allows a higher possibility of contact with the food than the gasket, the disc-shaped gasket/liner was selected, which allows a higher possibility of contact with the food and is thus more conservative in the assessment of the migration of the different plasticisers into the food.

Figure A 1. Example of variation of thickness in gasket along the diameter of the metal lid



Despite the choice of a regular shape (i.e., disc shape) in literature there is a large uncertainty related to the amount of plastisol used in a single metal lid. Therefore, to take into account this uncertainty, 3 different gasket mass values, reported in Table A 1, were retrieved from literature (Fankhauser-Noti Grob, 2006). A diameter of 44 mm was assumed for the 3 gaskets, based on the work of Fankhauser-Noti Grob, (2006), this choice is corroborated with the value range (e.g. from 38 mm to 82 mm) reported in a website of a gasket manufacturer. Finally, the density of the liner was assumed to be 833 kg/m^3, which was retrieved from the work of Bayer *et al.*, (1998).

With all this information the thicknesses for the three gaskets were calculated along with the corresponding volumes.

Table A 1. Gasket weight and corresponding estimated geometrical properties

Liner	Min	Mean	Max
Density [kg/m^3]	833		
Diameter [mm]	44		
Mass [mg]	95	281	450
Volume [mm^3]	114	337	540
Thickness [mm]	0.08	0.22	0.36

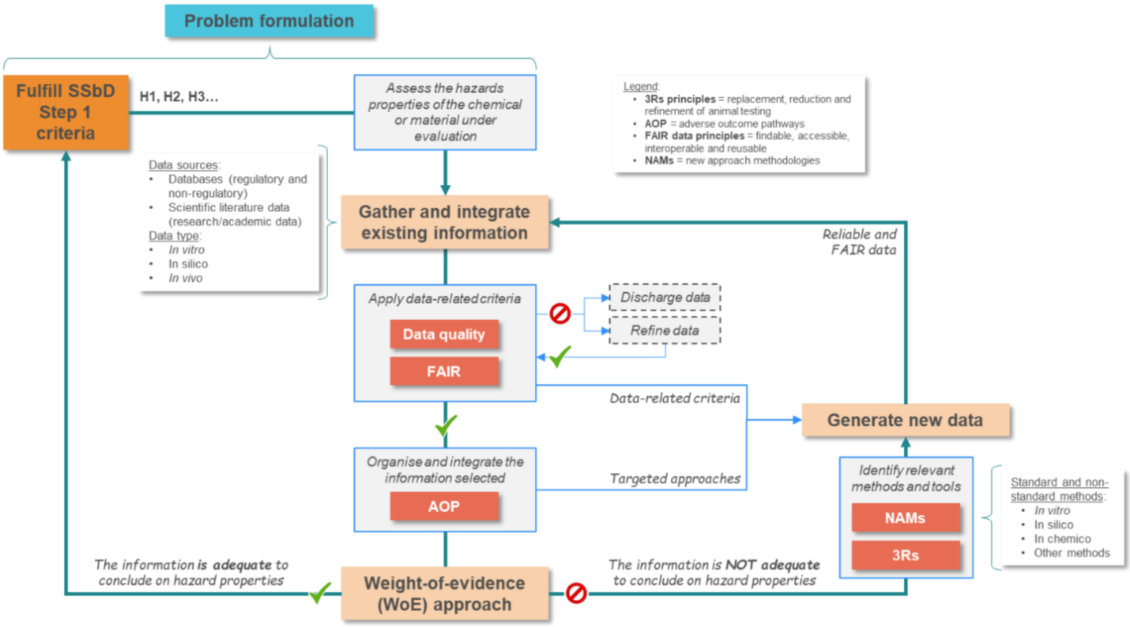
Annex 2. Integrated Approaches to Testing and Assessment (IATA)

The SSbD framework (Caldeira et al., 2022b) provides the setting to use 'integrated approaches to testing and assessment' (IATA). IATA are flexible approaches for chemical safety assessment based on the integration and translation of the data derived from multiple methods and sources. It relies on an integrated analysis of existing information coupled with the generation of new information using testing strategies. It follows an iterative approach to answer a defined question in a specific context, taking into account the acceptable level of uncertainty associated with the decision context (OECD, 2016, 2017b, 2020, 2023). In this context, the testing strategies to generate new information should prioritise the use of new approach methodologies (NAMs). The concept of NAMs is used as an umbrella for various approaches for generating data by using non-animal testing methods and technologies (Doak et al., 2022; ECHA, 2017a; Nymark et al., 2020). These methods include *in vivo, in vitro, in chemico, ex vivo, in silico* (computational) methods such as QSAR, grouping and read-across. IATA can also integrate high throughput methods (screening, imaging) or omics technologies (ECHA, 2017b). Several guidelines or tools to integrate such exist or under development (Hernández-Jerez et al., 2021; OECD, 2017a, 2017b, 2020).

For **Step 1** of the safety and sustainability assessment phase, an **IATA-like approach** is proposed in order to integrate data from various sources and methods (Figure A2) For each case study (*e.g. evaluating a single or a group of chemicals or materials*) the IATA guides the processes of data gathering, data generation and facilitates the conclusion regarding the hazard properties following a structured format.

The main component of the IATA includes the **problem formulation** (e.g. fulfilling hazard properties criteria as established by the SSbD framework as presented in the case study description) that requires the assessments of the possible hazard properties of a chemical or material (or group) and subsequent steps in order to fulfil them. These steps are referring to **gathering and assessing existing information** including a systematic data collection (from existing databases, literature review, etc.), application of data-related criteria (quality, FAIR (findable, accessible, interoperable and reusable), relevance, uncertainty analysis, etc.) before integration in the assessment. For the **integration and analysis of data**, the adverse outcome pathway (AOP) framework (OECD, 2017a) may be used to structure the available information. Using a **weight-of-evidence (WoE)** approach a conclusion (decision) can be taken regarding the criteria set-up in the 'problem formulation'. However, if the information is not adequate to make a conclusion, **additional data need to be generated**.

Figure A 2. Workflow proposed for the development of integrated approach to testing and assessment (IATA) in Step 1



Problem formulation

The approach on how to apply the proposed SSbD framework and the assessment steps will be defined by the problem formulation.

The problem formulation refers to the scope and goals in relation to the assessment, the level of uncertainty that is acceptable as well as the urgency of the assessment.

Problem formulation can be specific for example about a specific endpoint and hazard class in Step 1 or can be a general question in relation to a process in Step 2 that then, can have additional sub-questions.

Gathering existing information

The availability of data to be used for the assessment depends on the life cycle / development stage when the assessment is performed (e.g. less data will be available during the R&D phase, while more data will be available towards placing the chemical or material on the market). As such, the best available approach should be applied that allows screening for possible hazards properties e.g. at an early stage of the R&D process and require data gradually along the life cycle (Figure A 3). The SSbD framework will be a beneficiary of any high-quality data produced in other contexts (e.g. research and innovation, regulatory). Few examples are described in Table A 2.

Figure A 3. Examples of approach and cases regarding the data type and availability for Step 1, based on tools' availability and the life cycle of the chemicals or materials (examples A, B, C and D are detailed in Table below)

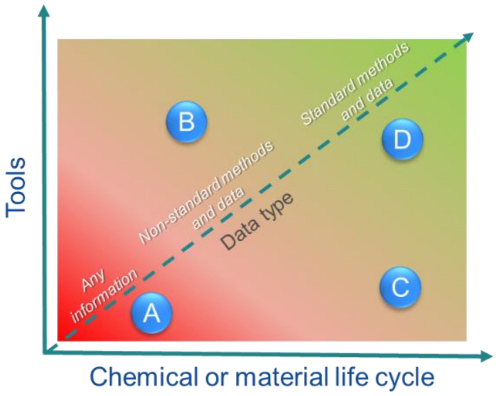


Table A 2. Examples of data-related situations for hazard assessment in SSbD Step 1

Example	Life cycle stage	Approach
Example A (early LC stage / no tools available)	Chemical in early phase of R&D	Use **any information available** (including from non-standardised NAMs, academic data, etc.) to evaluate and justify whether a conclusion can be made on a hazard endpoint with a sufficient level of confidence.
Example B (early LC stage / tools available)	Chemical in prototyping or production phase	If applicable, use first **standard methods to generate data** and if needed fill the data gaps with NAMs in an **integrated approach** (IATA, AOP) or any information available.
Example C (late LC stage / no tools available)	Chemical in use phase or EoL	Use of **weight of evidence (WoE) approach**, using data generated with NAMs (including non-standard methods) in an **integrated approach** (IATA, AOP) in order to evaluate and justify whether a hazard endpoint is fulfilled or not.
Example D (late LC stage / tools available)	Chemical in use phase or EoL	Use first **standard methods to generate data** and if needed fill the data gaps with NAMs or any information available.

Data from all possible sources should be used including non-regulatory or regulatory studies, and include *in vitro*, *in silico*, animal *in vivo* data, and epidemiological data or human data. In order to be considered in the SSbD context the information used should fulfil additional criteria regarding:

- Data quality, and
- FAIR principles (see (Krans et al., 2022) for examples of FAIR assessment tools that can be used).

If the data collected passes the two criteria it could be further organised and used for the assessment. For this step, the adverse outcome pathway (AOP) approach can be applied (see OECD, 2023; Vinken et al., 2017).

Weight-of-evidence (WoE) approach

The WoE approach (ECHA, 2016, 2017a, 2023b) is a way of considering all information available for an information requirement or (hazard) assessment. In a WoE approach, the information should be collected together, which may then suffice to allow for a conclusion to be made without further studies. The weight given to the available evidence depends on factors such as the quality of the data, consistency of results, nature and severity of effects and relevance of the information. Once existing data has been gathered, the WoE concept provides the opportunity to use any information or studies in order to make a conclusion on the hazard properties and fulfil the information requirements for Step 1.

The weight of evidence approach requires use of expert judgment and, therefore, it is essential to provide adequate and reliable documentation to make it transparent and understandable.

Generation of new data

The process of WoE is an iterative process linking the conclusion with the problem formulation and answering the question. If the question cannot be answered, then the WoE approach is the key to identify data needs and integrated testing strategies can be used to fill the data gaps, giving priority to NAMs for generating new information.

The goal is to fill the data gaps with high-quality and FAIR data towards a reliable and transparent SSbD assessment along the entire life cycle of the chemical or material:

- Identification of relevant tools and methods (in the cases where there are no tools available to generate data, this gap needs to be justified and described);
- Use of suitable and reliable new approach methodologies (NAMs), including non-standard methods, to generate data aligned to the 3Rs principles regarding replacement, reduction and refinement of animal testing;
- Use a targeted approach based on the knowledge gaps identified during the evaluation and integration of existing information;
- The experimental re-design based on testing (e.g. *in vitro*) and/or a non-testing method (e.g. *in silico*) need to consider whether the data generated will be FAIR.

Annex 3. Step 1 - Chemical information as input for Step 2

Table A 3. Physico-chemical and fate properties

Chemical name		**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Data source		https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15358/2/1	https://echa.europa.eu/registration-dossier/-/registered-dossier/13143/2/1	https://echa.europa.eu/registration-dossier/-/registered-dossier/15293/2/1	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15238/2/1	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/16022	https://echa.europa.eu/sl/registration-dossier/-/registered-dossier/15408
EC number		204-211-0	201-067-0	203-090-1	229-176-9	431-890-2	232-391-0
CAS number		117-81-7	77-90-7	103-23-1	6422-86-2	166412-78-8	08/07/8013
General	**Physical state at 20°C and 1013 hPa**	liquid	liquid	liquid	liquid	liquid	liquid
	Molecular weight (for assessment)	402.5	390.56	390.6	370	424.6	974.7
	Melting point at 101 325 Pa (°C)	-80	-50	-67.2	-67.8	-90	-2
	Vapour pressure (Pa)	0.0494	3.40E-05	1.00E-03	3.00E-05	0	8.40E-08
	Partition coefficient (Log Kow)	4.86	7.5	8.34	8.94	10	6.2
	Water solubility (µg/L)	4490	3	0.4	3.2	20	0.02
	Henry's law constant (in Pa m³/mol)	4.434	No data	No data	5.23	7.16	No data
Biodegradation	**Biodegradation in water: screening tests**	No clear answer (2x determined inherently biodegradable, 1x determined not readily biodegradable)	readily biodegradable	readily biodegradable	readily biodegradable	Results provided, but no summary	readily biodegradable
	Half-life in freshwater	No data	50 d at 12 °C	No data	No data	No data	No data
	Half-life in marine water	No data	No data	No data	No data	No data	No data
	Half-life in freshwater sediment	No data	300 d at 12 °C	No data	No data	No data	No data
	Half-life in soil	No data	300 d at 12 °C	No data	No data	Results provided, but no summary	No data
Bioaccumulation	**Bioaccumulation: BCF (aquatic species)**	31.57 L/kg ww	614	393 whole body ww	27 L/kg ww	189.3 (whole body ww)	No data
	Bioaccumulation: BMF in fish	No data	No data	No data	No data	No data	No data
	Bioaccumulation: BCF (terrestrial species)	No data	1	No data	No data	No data	No data

Chemical name		DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Abiotic degradation	**Degradation rate constant with OH radicals**	0 cm^3 molecule-1 d-1	No data	No data	No data	No data	No data
	Half-life in air (phototransformation)	1 d	No data	No data	No data	4.18 h	No data
	Half-life for hydrolysis	half-lives at pH 4: 3816 Years pH 7: 3.82 years pH 8: 139 days pH 9: 13.94 days (25°C each)	No data	Results for the preliminary test suggest that little, if any, hydrolysis occurs at the pH range of 4 to 9.	No data	Study performed, but no summary	No data
	Half-life in water (photolysis)	No data	No data	No data	No data	No data	No data
	Log Koc at 20 °C	4.27	6.10	5.43	4.56	6.59	10.00
	Log Kp (solids-water in soil) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in sediment) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in suspended matter) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in raw sewage sludge) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in settled sewage sludge) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in activated sewage sludge) in L/kg	No data	No data	No data	No data	No data	No data
	Log Kp (solids-water in effluent sewage sludge) in L/kg	No data	No data	No data	No data	No data	No data

Table A 4. Human Health Workers hazard information

Hazards for workers							
		DEHP	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Hazard via Inhalation route	**Systemic effects – long term exposure (DNEL mg/m³)**	1.6	7.04	17.8	23.2	235/35	11.9
	Systemic effects – acute exposure (DNEL mg/m³)	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	70
	Local effects – long term exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
	Local effects – acute exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
Hazard via Dermal route	**Systemic effects – long term exposure (DNEL in mg/kg bw/day)**	3.4	2	25.5	6.58	42	1.7
	Systemic effects – acute exposure (DNEL in mg/kg bw/day)	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	10
	Local effects – long term exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
	Local effects – acute exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
Hazard for the Eyes	**Local effects**	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified

Table A 5. Human Health Consumers hazard information

Hazards for consumers							
		DEHP	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**
Hazard via Inhalation route	**Systemic effects – long term exposure (DNEL mg/m^3)**	0.13	1.74	4.4.	6.86	70/25	2.8
	Systemic effects – acute exposure (DNEL mg/m^3)	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	17.5
	Local effects – long term exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
	Local effects – acute exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
Hazard via Dermal route	**Systemic effects – long term exposure (DNEL in mg/kg bw/day)**	0.72	1	13	3.95	25	0.8
	Systemic effects – acute exposure (DNEL in mg/kg bw/day)	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	5
	Local effects – long term exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
	Local effects – acute exposure	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified
Hazard via Oral route	**Systemic effects – long term exposure (DNEL in mg/kg bw/day)**	0.036	1	1.3	3.95	2	0.8
Hazard for the Eyes	**Local effects**	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified	No hazard identified

Annex 4. Step 2 and 3- Plasticiser Life Cycle and Relevant Contributing Scenarios

Table A 6. Individual amended values - Substance Data used for Risk Assessment

	DEHP	**DEHA**	**ATBC**	**DINCH**	**ESBO**	**DEHT**
Smiles code	CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	CCCC[C@@H](CC)COC(=O)CCCCC(=O)OC[C@H](CC)CCCC	CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC	CC(C)CCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC(C)C	CCCCCC1OC1CC1OC1CCCCCCCC(=O)OCC(COC(=O)CCCCCCCC1OC1CC1OC1CCCCC)OC(=O)CCCCCCCC1OC1CC1OC1CCCCC	CCCCC(CC)COC(=O)c1ccc(cc1)C(=O)OCC(CC)CCCC
Physical-Chemical Data						
Vapour pressure [37]	0.000000001 at 25 °C	0.000000001 at 25 °C			0.000000001 at 25 °C	
Henry's law constant (in Pa m³/mol) [38]	0.01317225 at 25 °C	0.0439751 at 25 °C	4.434 at 25 °C			1.033515 at 25°C
Environmental Fate Endpoints						
Biodegradation in water: screening tests			Assume inherently biodegradable	Assume not readily biodegradable		
PBT assessment			Set to not PBT to allow PEC calculations in Chesar			
Freshwater [39]	PNEC = 1.90E-05 mg/L			PNEC = 2.24E-6 mg/L	PNEC = 2.10E-09 mg/L	
STP [40]					PNEC = 2.10E-09 mg/L	

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[37] The lowest value accepted by SimpleTreat 4.1 was used instead of 0

[38] Conversion factor from atm m³/mol of 101325 was used

[39] Lowest chronic value for freshwater species from Ecosar, based on Smiles codes, with AF = 10; as opposed to the previous assumption that no hazard can be identified, these substances all show very low PNEC values for surface water

[40] Set to the same value as PNEC surface water

Table A 7. QSAR Substance Data used for alternative Risk Assessment

	DEHP	**DEHA**	**ATBC**	**DINCH**	**ESBO**	**DEHT**
Smiles code	CCCCC(CC)COC(=O)c1ccccc1C(=O)OCC(CC)CCCC	CCCC[C@@H](CC)COC(=O)CCCCC(=O)OC[C@H](CC)CCCC	CCCCOC(=O)CC(CC(=O)OCCCC)(OC(C)=O)C(=O)OCCCC	CC(C)CCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC(C)C	CCCCCC1OC1CC1OC1CCCCCCCC(=O)OCC(COC(=O)CCCCCCCC1OC1CC1OC1CCCCC)OC(=O)CCCCCCCC1OC1CC1OC1CCCCC	CCCCC(CC)COC(=O)c1ccc(cc1)C(=O)OCC(CC)CCCC
Molecular weight (g/mol) [41]	390.57	370.58	402.42	424.67	975.41	390.57
Physical-Chemical Data						
Mean melting point (°C) [42]	63.87	8.96	94.35	53.84	349.84	63.87
Vapor Pressure (Modified Grain Method; Pa at 25°C) [43]	0.0027	0.000427	0.000607	0.000128	1.60E-20	0.00286
Log Kow [44]	8.39	8.12	4.29	9.82	14.84	8.39
Water solubility (mg/L at 25°C) [45]	0.001132	0.0005452	0.6464	8.83E-06	1.03E-13	0.0002387
Henry's law constant (in Pa	933.80	290.00	3.78E-01	6170.00	1.52E-04	4668.00

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[41] EPISUITE
[42] MPBPVP v1.43
[43] MPBPVP v1.43
[44] KOWWIN v1.68
[45] WSKOW v1.42

	DEHP	DEHA	ATBC	DINCH	ESBO	DEHT
m³/mol at 25°C) [46]						
Other parameters needed for the risk assessment						
Ready Biodegradability Prediction [47]	Yes	Yes	Yes	No	No	Yes
Log Koc [48]	99470	192900	1468	1681000	287600000	272100
PBT assessment [49]	not P not B vT	not P B	not P not B not T	not P B	not P B	not P B not T
PNEC freshwater (mg/L) [50]	1.900E-05	2.770E-05	1.160E-02	2.240E-06	2.100E-09	1.900E-05
PNEC sediment (mg/kg dwt) [51]	6.36E-05	9.28E-05	1.74E+00	7.50E-06	7.03E-09	6.36E-05
PNEC STP (mg/L) [52]	1.900E-05	2.770E-05	1.160E-02	2.240E-06	2.100E-09	1.900E-05
PNEC soil (mg/kg dwt) [53]	4.14E-06	5.05E-06	3.38E-01	1.14E-06	3.49E-10	8.09E-06

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[46] VP/WSol estimate

[47] BIOWIN v4.10; where the prediction is “no”, inherent biodegradability was assumed.

[48] KOCWIN v2.00

[49] For all substances, the Chesar assessment assumes that they are not PBT

[50] ECOSAR v1.11 Class-specific Estimations, lowest chronic value for freshwater species with AF = 10

[51] EPM

[52] Set to the same value as PNEC surface water

[53] EPM

Annex 5. Step 2 – Exposure estimations and RCR for workers

Table A 8. Operational conditions and Risk Management Measures.

MANUFACTURE OF PLASTICISER
Product (article) characteristics
• Percentage (w/w) of substance in mixture/article: <= 100 %
• Physical form of the used product: Liquid, including paste/slurry/suspension
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 8 h/day
Technical and organisational conditions and measures
• Local exhaust ventilation: No
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes (effectiveness >= 80%)
• Respiratory protection: No
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 40 °C

Table A 9. Exposure estimations and RCR for workers

MANUFACTURE OF PLASTICISER												
Route of exposure and type of effects	**DEHP**		**DEHA**		**DEHT**		**DINCH**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
SCC Production (PROC 1)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	0.117	0.017
Dermal, systemic, long term (mg/kg bw/day)	6.8E-3	< 0.01	6.8E-3	< 0.01	6.8E-3	< 0.01	6.8E-3	< 0.01	6.8E-3	< 0.01	6.8E-3	< 0.01
Combined routes, systemic, long-term		< 0.01		< 0.01		< 0.01		< 0.01		< 0.01		0.02
Continuous synthesis (PROC 2)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	11.74	1.668
Dermal, systemic, long term (mg/kg bw/day)	0.274	0.081	0.274	0.011	0.274	0.042	0.274	< 0.01	0.274	0.161	0.274	0.137
Combined routes, systemic, long-term		0.081		0.011		0.059		< 0.01		0.161		1.805
Batch synthesis (PROC 3)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	0.138	0.041	0.138	< 0.01	0.138	0.021	0.138	< 0.01	0.138	0.081	0.138	0.069
Combined routes, systemic, long-term		0.041		< 0.01		0.039		< 0.01		0.081		3.041
Non-SCC Production (PROC 4)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	1.372	0.404	1.372	0.054	1.372	0.209	1.372	0.033	1.372	0.807	1.372	0.686
Combined routes, systemic, long-term		0.404		0.054		0.226		0.033		0.807		3.658
Transfer, non-dedicated facility (PROC 8a)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	2.742	0.806	2.742	0.108	2.742	0.417	2.742	0.065	2.742	1.613	2.742	1.371
Combined routes, systemic, long-term		0.806		0.108		0.435		0.065		1.613		4.343
Transfer, dedicated facility (PROC 8b)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	2.742	0.806	2.742	0.108	2.742	0.417	2.742	0.065	2.742	1.613	2.742	1.371
Combined routes, systemic, long-term		0.806		0.108		0.435		0.065		1.613		4.343

MANUFACTURE OF PLASTICISER												
Route of exposure and type of effects	**DEHP**		**DEHA**		**DEHT**		**DINCH**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Filling into small containers (PROC 9)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	1.372	0.404	1.372	0.054	1.372	0.209	1.372	0.033	1.372	0.807	1.372	0.686
Combined routes, systemic, long-term		0.404		0.054		0.226		0.033		0.807		3.658
Laboratory/Quality Control Operations (PROC 15)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	5.87	0.834
Dermal, systemic, long term (mg/kg bw/day)	0.068	0.02	0.068	< 0.01	0.068	0.01	0.068	< 0.01	0.068	0.04	0.068	0.034
Combined routes, systemic, long-term		0.02		< 0.01		0.015		< 0.01		0.04		0.868

Table A 10. Operational conditions and Risk Management Measures

FORMULATION OF A PLASTISOL
Product (article) characteristics
• Percentage (w/w) of substance in mixture/article: <= 100 %
• Physical form of the used product: Liquid, including paste/slurry/suspension
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 8 h/day
Technical and organisational conditions and measures
• Local exhaust ventilation: Yes, basic LEV such as canopy hood, movable capturing hood or other multi-purpose LEV (assumed effectiveness 50-80%)
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes (effectiveness >= 80%)
• Respiratory protection: No
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 40 °C

Table A 11. Exposure estimations and RCR for workers

FORMULATION OF A PLASTISOL												
Route of exposure and type of effects	**DEHP**		**DEHA**		**DEHT**		**DINCH**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Handling of Small Containers Containing Additive (PROC 9)												
Inhalation, systemic, long term (mg/m^3)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	1.372	0.404	1.372	0.054	1.372	0.209	1.372	0.033	1.372	0.807	1.372	0.686
Combined routes, systemic, long-term		0.404		0.054		0.226		0.033		0.807		3.658
Handling Large Containers Containing Additive (PROC 8b)												
Inhalation, systemic, long term (mg/m^3)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	2.742	0.806	2.742	0.108	2.742	0.417	2.742	0.065	2.742	1.613	2.742	1.371

FORMULATION OF A PLASTISOL												
Route of exposure and type of effects	**DEHP**		**DEHA**		**DEHT**		**DINCH**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Combined routes, systemic, long-term		0.806		0.108		0.435		0.065		1.613		4.343
Continuous Mixing Process (PROC 4) (Operating temperature <= 60 °C)												
Inhalation, systemic, long term (mg/m³)	1.139	0.712	1.08E3	60.62	1.14E3	49.10	1.24E3	5.27	2.84E3	238.7	1.17E3	166.7
Dermal, systemic, long term (mg/kg bw/day)	1.372	0.404	1.372	0.054	1.372	0.209	1.372	0.033	1.372	0.807	1.372	0.686
Combined routes, systemic, long-term		1.115		60.68		49.31		5.303		239.5		167.4
Batch Mixing Process (PROC 5) (Operating temperature <= 60 °C)												
Inhalation, systemic, long term (mg/m³)	1.139	0.712	2.7E3	151.5	2.85E3	122.7	3.1E3	13.17	7.1E3	596.8	2.93E3	416.8
Dermal, systemic, long term (mg/kg bw/day)	2.742	0.806	2.742	0.108	2.742	0.417	2.742	0.065	2.742	1.613	2.742	1.371
Combined routes, systemic, long-term		1.518		151.6		123.1		13.24		598.4		418.2
Laboratory/Quality Control Operations (PROC 15) (Dermal protection >= 95%)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	5.87	0.834
Dermal, systemic, long term (mg/kg bw/day)	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	0.01	0.017	< 0.01
Combined routes, systemic, long-term		< 0.01		< 0.01		< 0.01		< 0.01		0.01		0.842

Table A 12. Operational conditions and Risk Management Measures

PRODUCTION OF SEALING GASKET
Product (article) characteristics
• Percentage (w/w) of substance in mixture/article: <= 33.3 %
• Physical form of the used product: Solid (material with no or very low dustiness)
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 8 h/day
Technical and organisational conditions and measures
• Local exhaust ventilation: Yes, basic LEV such as canopy hood, movable capturing hood or other multi-purpose LEV (assumed effectiveness 50-80%)
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes (effectiveness >= 80%)
• Respiratory protection: No
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 40 °C

Table A 13. Exposure estimations and RCR for workers

PRODUCTION OF SEALING GASKET												
Route of exposure and type of effects	**DEHP**		**DEHA**		**DEHT**		**DINCH**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Handling of Small Containers Containing Additive (PROC 9)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	1.372	0.404	1.372	0.054	1.372	0.209	1.372	0.033	1.372	0.807	1.372	0.686
Combined routes, systemic, long-term		0.404		0.054		0.226		0.033		0.807		3.658
Handling Large Containers Containing Additive (PROC 8b)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.414	0.018	9.91E-3	< 0.01	0	< 0.01	20.92	2.972
Dermal, systemic, long term (mg/kg bw/day)	2.742	0.806	2.742	0.108	2.742	0.417	2.742	0.065	2.742	1.613	2.742	1.371
Combined routes, systemic, long-term		0.806		0.108		0.435		0.065		1.613		4.343
Use in a Closed and/or Semi-Open Converting Process (e.g. Extrusion, injection) (PROC 14) (Operating temperature <= 200 °C)												
Inhalation, systemic, long term (mg/m³)	56.95	35.59	2.7E3	151.5	2.85E3	122.7	3.1E3	13.17	7.1E3	596.8	2.93E3	416.8
Dermal, systemic, long term (mg/kg bw/day)	0.686	0.202	0.686	0.027	0.686	0.104	0.686	0.016	0.686	0.404	0.686	0.343
Combined routes, systemic, long-term		35.8		151.5		122.8		13.19		597.2		417.2
Use in an Open Converting Process (e.g. Calendering) (PROC 6) (Operating temperature <= 200 °C)												
Inhalation, systemic, long term (mg/m³)	56.95	35.59	1.079	0.061	1.139	0.049	1.238	< 0.01	2.841	0.239	58.69	8.338
Dermal, systemic, long term (mg/kg bw/day)	5.486	1.614	5.486	0.215	5.486	0.834	5.486	0.131	5.486	3.227	5.486	2.743
Combined routes, systemic, long-term		37.21		0.276		0.883		0.136		3.466		11.08
Roll and spread coating (PROC 10) (Operating temperature <= 200 °C)												
Inhalation, systemic, long term (mg/m³)	113.9	71.19	2.7E3	151.5	2.85E3	122.7	3.1E3	13.17	7.1E3	596.8	2.93E3	416.8
Dermal, systemic, long term (mg/kg bw/day)	5.486	1.614	5.486	0.215	5.486	0.834	5.486	0.131	5.486	3.227	5.486	2.743
Combined routes, systemic, long-term		72.80		151.7		123.5		13.30		600.1		419.6
Laboratory/Quality Control Operations (PROC 15) (Dermal protection >= 95 %)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	5.87	0.834
Dermal, systemic, long term (mg/kg bw/day)	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	0.01	0.017	< 0.01
Combined routes, systemic, long-term		< 0.01		< 0.01		< 0.01		< 0.01		0.01		0.842

Table A 14. Revised Operational conditions and RMMs in the manufacturing process.

MANUFACTURE OF PLASTICISER
Product (article) characteristics
• Percentage (w/w) of substance in mixture/article: <= 100 %
• Physical form of the used product: Liquid, including paste/slurry/suspension
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 4 h/day
Technical and organisational conditions and measures
• Local exhaust ventilation: No
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: No
• Respiratory protection: No
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 25 °C

Table A 15. RCR for the manufacture of plasticisers considering a set of additional measures to mitigate the risk

Chemical production or refinery in closed process without likelihood of exposure or processes with equivalent containment conditions (PROC 1)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.074	< 0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	0.07	0.01
Dermal, systemic, long term (mg/kg bw/day)	0.034	< 0.01	3.4E-3	< 0.01	0.034	0.01	0.034	< 0.01	0.034	0.02	0.034	0.017
Combined routes, systemic, long-term		< 0.01		< 0.01		0.053		< 0.01		0.034		0.027
Chemical production or refinery in closed continuous process with occasional controlled exposure or processes with equivalent containment conditions (PROC 2)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743)	< 0.01	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	0.07	0.01
Dermal, systemic, long term (mg/kg bw/day)	1.37	0.033	1.37	0.054	1.37	0.403	1.37	0.208	1.37	0.806	0.034	0.017
Combined routes, systemic, long-term		0.036		0.09		0.83		0.238		0.949		0.027
Manufacture or formulation in the chemical industry in closed batch processes with occasional controlled exposure or processes with equivalent containment conditions (PROC 3)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.647	0.036	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	2.113	0.3
Dermal, systemic, long term (mg/kg bw/day)	1.37	0.054	0.69	0.027	0.69	0.203	0.69	0.105	0.69	0.406	0.69)	0.345
Combined routes, systemic, long-term		0.09		0.063		0.63		0.134		0.549		0.645
Chemical production where opportunity for exposure arises (PROC 4)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743	< 0.01	0.743	< 0.01	0.683	0.427	0.684	0.029	1.706	0.143	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	0.69	0.016	6.86	0.163	0.686	0.202	0.686	0.104	0.686	0.404	0.686	0.343
Combined routes, systemic, long-term		0.02		0.166		0.629		0.134		0.549		0.843
Transfer of substance or mixture (charging and discharging) at non-dedicated facilities (PROC 8a)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	

	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743	0.01	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	7.044	1.001
Dermal, systemic, long term (mg/kg bw/day)	13.71	0.326	13.71	0.538	1.371	0.403	1.371	0.208	1.371	0.806	1.371	0.686
Combined routes, systemic, long-term		0.33		0.574		0.83		0.238		0.949		1.686
Transfer of substance or mixture (charging and discharging) at dedicated facilities (PROC 8b)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743	< 0.01	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	1.761	0.25
Dermal, systemic, long term (mg/kg bw/day)	13.71	0.326	13.71	0.538	1.371	0.403	1.371	0.208	1.371	0.806	1.371	0.686
Combined routes, systemic, long-term		0.33		0.574		0.83		0.238		0.949		0.936
Transfer of substance or mixture into small containers (dedicated filling line, including weighing) (PROC 9)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743	< 0.01	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	6.8	0.163	6.86	0.269	0.686	0.202	0.686	0.404	0.686	0.404	0.343	0.172
Combined routes, systemic, long-term		0.166		0.305		0.629		0.547		0.547		0.672
Use as laboratory reagent (PROC 15)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.743	< 0.01	0.647	0.036	0.683	0.427	0.684	0.029	1.706	0.143	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	0.34	< 0.01	0.34	0.013	0.34	0.1	0.34	0.052	0.34	0.2	0.34	0.17
Combined routes, systemic, long-term		0.011		0.05		0.527		0.081		0.343		0.67

Table A 16. Revised Operational conditions and RMMs in the formulation of plastisol

FORMULATION OF A PLASTISOL
Product (article) characteristics
• Percentage (w/w) of substance in mixture/article: <= 30 %
• Physical form of the used product: Liquid, including paste/slurry/suspension
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 4 h/day
Technical and organisational conditions and measures
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
• Local exhaust ventilation: No
Conditions and measures related to personal protection, hygiene and health evaluation
• Respiratory protection: Yes (APF >= 10)
• Dermal protection: Chemical resistant dermal protection with basic employee training. (effectiveness >= 90%)
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 25 °C

Table A 17. RCR for the Formulation of Plastisol considering a set of additional measures to mitigate the risk

Batch Mixing Process (PROC 5)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.074	< 0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	1.371	0.033	1.371	0.054	1.371	0.403	1.371	0.208	1.371	0.806	1.371	0.686
Combined routes, systemic, long-term		0.033		0.057		0.446		0.211		0.82		1.186
Transfer of substance or mixture (charging and discharging) at non-dedicated facilities (PROC 8a)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.744	< 0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	1.371	0.033	1.371	0.054	1.371	0.403	1.371	0.208	1.371	0.806	1.371	0.686
Combined routes, systemic, long-term		0.033		0.057		0.446		0.211		0.82		1.186
Transfer, dedicated facility (PROC 8b)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		ATBC	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	Exposure	RCR
Inhalation, systemic, long term (mg/m³)	0.744	< 0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	7.044	1.001
Dermal, systemic, long term (mg/kg bw/day)	1.371	0.033	1.371	0.054	1.371	0.403	1.371	0.208	1.371	0.806	1.371	0.686
Combined routes, systemic, long-term		0.033		0.057		0.446		0.211		0.82		1.686
Small Containers Containing Additive (PROC 9)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.074	0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	3.522	0.5
Dermal, systemic, long term (mg/kg bw/day)	0.686	0.016	0.686	0.027	0.686	0.202	0.686	0.104	0.686	0.404	0.686	0.343
Combined routes, systemic, long-term		0.017		0.031		0.244		0.107		0.418		0.843
Laboratory/Quality Control Operations (PROC 15) (Dermal protection >= 95%)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	5.87	0.834
Dermal, systemic, long term (mg/kg bw/day)	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	0.01	0.017	< 0.01
Combined routes, systemic, long-term		< 0.01		< 0.01		< 0.01		< 0.01		0.01		0.842

Table A 18. Revised Operational conditions and RMMs in the production of sealing gasket

PRODUCTION OF SEALING GASKET
Product (article) characteristics
• Physical form of the used product: Liquid, including paste/slurry/suspension
• Percentage (w/w) of substance in mixture/article: <= 30 %
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: <= 4 h/day
Technical and organisational conditions and measures
• Occupational Health and Safety Management System: Advanced
• Room ventilation: Good (3 to 5 ACH)
• Local exhaust ventilation: Yes, specifically designed fixed capturing hood, on tool extraction or enclosing hoods (assumed effectiveness >= 90-95%)
Conditions and measures related to personal protection, hygiene and health evaluation
• Respiratory protection: No
• Dermal protection: Chemical resistant dermal protection with basic employee training. (effectiveness >= 90%)
• Face/eye protection: No
Other conditions affecting workers exposure
• Place of use: Indoor
• Operating temperature: <= 25 °C

Table A 19. RCR for the production of sealing gasket considering a set of additional measures to mitigate the risk

Use in Roll and/or Spread Coating (PROC 10)												
Route of exposure and type of effects	**DINCH**		**DEHA**		**DEHP**		**DEHT**		**ESBO**		**ATBC**	
	Exposure	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**	**Exposure**	**RCR**
Inhalation, systemic, long term (mg/m³)	0.074	< 0.01	0.065	< 0.01	0.068	0.043	0.068	< 0.01	0.171	0.014	0.704	0.1
Dermal, systemic, long term (mg/kg bw/day)	2.743	0.065	0.686	0.027	2.743	0.807	2.743	0.417	2.743	1.614	1.372	0.686
Combined routes, systemic, long-term		0.066		0.031		0.849		0.42		1.628		0.786
Laboratory/Quality Control Operations (PROC 15) (Dermal protection >= 95 %)												
Inhalation, systemic, long term (mg/m³)	0	< 0.01	0	< 0.01	0.114	< 0.01	9.91E-3	< 0.01	0	< 0.01	5.87	0.834
Dermal, systemic, long term (mg/kg bw/day)	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	< 0.01	0.017	0.01	0.017	< 0.01
Combined routes, systemic, long-term		< 0.01		< 0.01		< 0.01		< 0.01		0.01		0.842

Annex 6. Step 2 and 3 – RCR for the Environment

Table A 20. RCRs for ERC 1. Manufacturing process

Protection target	DEHP	DEHA	ATBC	DINCH	ESBO	DEHT
Fresh water	RCR = 3.78E4	RCR = 2.42E4	RCR = 438.9	RCR = 1.6E5	RCR = 7.63E4	RCR = 1.9E4
Sediment (freshwater)	RCR = 1.08E3	RCR = 848.2	RCR = 435.1	RCR = 1.63E6	RCR = 1.6E6	RCR = 4.95E3
Marine water			RCR = 482.8			RCR = 1.9E4
Sediment (marine water)	RCR = 537.6		RCR = 435.1			RCR = 4.95E3
Sewage Treatment Plant	RCR = 0.116	RCR = 20.36	RCR = 0.992	RCR = 1.11E7	RCR = 2.4E10	RCR = 21.35
Agricultural soil	RCR = 148.0	RCR = 1.53E3	RCR = 635.6	RCR = 258.4	RCR = 1.88E3	RCR = 4.78E6
Predator's prey (freshwater)	RCR = 18.33		RCR = 0.04		Qualitative risk	RCR = 1.557
Predator's prey (marine water)	RCR = 1.837		RCR < 0.01		Qualitative risk	RCR = 0.156
Top predator's prey (marine water)	RCR = 0.374		RCR < 0.01		Qualitative risk	RCR = 0.031
Predator's prey (terrestrial)	RCR = 22.18		RCR = 5.354		Qualitative risk	RCR = 27.21

Table A 21. RCRs for ERC 2. Plastisol Formulation

Protection target	DEHP	DEHA	ATBC	DINCH	ESBO	DEHT
Fresh water	RCR = 1.26E4	RCR = 8.06E3	RCR = 146.3	RCR = 5.34E4	RCR = 2.55E4	RCR = 6.34E3
Sediment (freshwater)	RCR = 358.5	RCR = 283.1	RCR = 145.1	RCR = 5.44E5	RCR = 5.36E5	RCR = 1.65E3
Marine water			RCR = 161.0			RCR = 6.34E3
Sediment (marine water)	RCR = 179.4		RCR = 145.1			RCR = 1.65E3
Sewage Treatment Plant	RCR = 0.039	RCR = 6.787	RCR = 0.331	RCR = 3.71E6	RCR = 8E9	RCR = 7.118
Agricultural soil	RCR = 49.36	RCR = 511.2	RCR = 211.9	RCR = 86.16	RCR = 634.9	RCR = 1.59E6
Predator's prey (freshwater)	RCR = 6.145		RCR = 0.013		Qualitative risk	RCR = 0.521
Predator's prey (marine water)	RCR = 0.617		RCR < 0.01		Qualitative risk	RCR = 0.052
Top predator's prey (marine water)	RCR = 0.13		RCR < 0.01		Qualitative risk	RCR = 0.011
Predator's prey (terrestrial)	RCR = 7.401		RCR = 1.785		Qualitative risk	RCR = 9.075

Table A 22. RCRs for ERC 5. Metal cap liner production

Protection target	DEHP	DEHA	ATBC	DINCH	ESBO	DEHT
Fresh water	RCR = 3.15E5	RCR = 2.01E5	RCR = 3.66E3	RCR = 1.33E6	RCR = 6.35E5	RCR = 1.58E5
Sediment (freshwater)	RCR = 8.96E3	RCR = 7.06E3	RCR = 3.62E3	RCR = 1.36E7	RCR = 1.33E7	RCR = 4.12E4
Marine water			RCR = 4.02E3			RCR = 1.58E5
Sediment (marine water)	RCR = 4.48E3		RCR = 3.62E3			RCR = 4.12E4
Sewage Treatment Plant	RCR = 0.966	RCR = 169.6	RCR = 8.27	RCR = 9.28E7	RCR = 2E11	RCR = 177.9
Agricultural soil	RCR = 1.23E3	RCR = 1.28E4	RCR = 5.3E3	RCR = 2.15E3	RCR = 1.56E4	RCR = 3.98E7
Predator's prey (freshwater)	RCR = 152.4		RCR = 0.331		Qualitative risk	RCR = 12.95
Predator's prey (marine water)	RCR = 15.24		RCR = 0.033		Qualitative risk	RCR = 1.295
Top predator's prey (marine water)	RCR = 3.056		RCR < 0.01		Qualitative risk	RCR = 0.259
Predator's prey (terrestrial)	RCR = 184.9		RCR = 44.61		Qualitative risk	RCR = 226.7

Table A 23. RCRs for ERC 11a. FCM application

Protection target	DEHP	DEHA	ATBC	DINCH	ESBO	DEHT
Fresh water	RCR = 13.80	RCR = 18.56	RCR = 0.125	RCR = 80.95	RCR = 114.7	RCR = 5.806
Sediment (freshwater)	RCR = 0.393	RCR = 0.652	RCR = 0.124	RCR = 824.2	RCR = 2.41E3	RCR = 1.51
Marine water			RCR = 0.129			RCR = 6.113
Sediment (marine water)	RCR = 0.313		RCR = 0.117			RCR = 1.59
Sewage Treatment Plant	RCR < 0.01	RCR < 0.01	RCR < 0.01	RCR = 5.105	RCR = 1.1E4	RCR < 0.01
Agricultural soil	RCR < 0.01	RCR = 0.064	RCR < 0.01	RCR < 0.01	RCR = 12.47	RCR = 49.14
Predator's prey (freshwater)	RCR = 0.049		RCR < 0.01		Qualitative risk	RCR < 0.01
Predator's prey (marine water)	RCR < 0.01		RCR < 0.01		Qualitative risk	RCR < 0.01
Top predator's prey (marine water)	RCR < 0.01		RCR < 0.01		Qualitative risk	RCR < 0.01
Predator's prey (terrestrial)	RCR < 0.01		RCR < 0.01		Qualitative risk	RCR < 0.01

Table A 24. RCRs for ERC 10a. FCM application

Protection target	**DEHP**	**DEHA**	**ATBC**	**DINCH**	**ESBO**	**DEHT**
Fresh water	RCR = 14.9	RCR = 19.26	RCR = 0.138	RCR = 85.57	RCR = 116.9	RCR = 6.355
Sediment (freshwater)	RCR = 0.424	RCR = 0.676	RCR = 0.136	RCR = 871.3	RCR = 2.46E3	RCR = 1.653
Marine water			RCR = 0.143			RCR = 6.662
Sediment (marine water)	RCR = 0.328		RCR = 0.129		RCR = 7.04E5	RCR = 1.733
Sewage Treatment Plant	RCR < 0.01	RCR < 0.01	RCR < 0.01	RCR = 326.7	RCR = 12.52	RCR < 0.01
Agricultural soil	RCR < 0.01	RCR = 0.109	RCR = 0.02	RCR = 0.014	Qualitative risk	RCR = 187.1
Predator's prey (freshwater)	RCR = 0.051		RCR < 0.01		Qualitative risk	RCR < 0.01
Predator's prey (marine water)	RCR < 0.01		RCR < 0.01		Qualitative risk	RCR < 0.01
Top predator's prey (marine water)	RCR < 0.01		RCR < 0.01		Qualitative risk	RCR < 0.01
Predator's prey (terrestrial)	RCR < 0.01		RCR < 0.01		RCR < 0.01	RCR < 0.01

Annex 7. Step 4 - Life cycle inventories

A7.1 Raw Material Acquisition and pre-processing

This life cycle stage includes the production of all the raw materials needed for the manufacturing of the gasket, namely the different plasticisers, the PVC and the additives. Below the production of the different plasticisers and its LCA modelling is described, as well as which modelling choice are used for the PVC and the additives.

Di-(2-ethyl hexyl) Phthalate – DEHP

The production of DEHP is made through esterification of Ethyl hexanol and phthalic anhydride as it is explained in section 2.1.2. The LCA model for the DEHP production has been built using stoichiometric quantity for the precursors and data extracted from the DINP ecoprofile (ECPI, 2015) to model the energy requirement and the water balance. The catalyst quantity is considered in the cut-off. Using stoichiometric quantities does not account for reaction losses. This is a limitation due to the lack of information. However, this assumption is kept consistently across all the other plasticiser models.

The transport of the raw materials is modelled considering the default distances for Europe recommended in PEF method.

Table A 25 and Table A 26 summarise the input and output for the DEHP production unit process. For each data the information source is provided in column "Dataset". Unless otherwise specified, dataset from ecoinvent v3.6 (Wernet et al. 2016) is used.

Table A 25. Life cycle inventory of the raw materials required for 1 kg of DEHP

Inventory data		Quantity	Unit	Dataset
Raw materials	Phthalic anhydride	0.379	kg	Phthalic anhydride {RER}| production | APOS, U
	2-ethyl hexanol	0.667	kg	See Table A 27
Transport	Ship	0.282	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.251	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.136	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table A 26. Life cycle inventory for the production of 1 kg of DEHP

Inventory data		Quantity	Unit	Dataset
Input	Heat	0.97	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Deionised water	0.14	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
	Process water	0.004	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Output	Wastewater to WWTP	0.15	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U
	Water from cooling	8.5	kg	Water, Europe without Switzerland
	Water vapour	0.35	kg	-

The synthesis of the two precursors reported in Table A 25 is also briefly described below since it is a relevant part of the life cycle and to show the rationale behind the modelling choices, either when they are part of the foreground system or they are modelled with secondary data. In particular, the 2-ethyl hexanol was modelled from literature data since no similar processes were found in the ecoinvent database.

Synthesis of phthalic anhydride

There are two main pathways to produce phthalic anhydride, the oldest and less relevant is through the oxidation of naphthalene, the newest and most relevant is the oxidation of ortho-xylene. The first process has declined in popularity in the last decades since the naphthalene has been available in limited quantity as a by-product of the coke production (Lorz et al., 2007), while the o-xylene is a largely available chemical. For the purpose of the present study, due to its relevance, the production of phthalic anhydride from the oxidation of o-xylene route is considered, using the ecoinvent dataset for phthalic anhydride production in Europe.

Synthesis of 2-ethyl hexanol

2-Ethyl hexanol is one of the most relevant alcohols produced globally. Mostly used for the synthesis of plasticisers, with a volume of over 4 million tons per year (AgileIntel Research, 2022). The industrial production has two main feedstock: butyraldehyde or acetaldehyde. The latter is not relevant due to its higher cost compared to butyraldehyde. Therefore, the most relevant route nowadays is via the condensation of butyraldehyde, which is derived from a refinery process called oxo-synthesis involving the use of syngas and propylene (Raff, 2013).

2-Ethyl hexanol is produced in four steps:

1. The butyraldehyde undergoes a condensation reaction catalysed by a sodium hydroxide solution, and produces ethylhexanal and water. The ratio of butyraldehyde to aqueous solution is in the range 1:10 - 1:20.
2. The alkali solution and the organic phase spontaneously separate in a separation drum. After the separation, part of the aqueous solution exits the process to eliminate the additional water produced in the reaction.
3. The hydrogenation of the unsaturated 2-ethyl-2-hexenal reaction is performed in one or more fixed catalyst bed reactors, and heat of reaction is used to produce steam.
4. The final product is then separated from impurities with a set of distillation columns (Bahrmann et al., 2013).

The two reactions (step 1 and 3) do not require external energy since they are both exothermic, the only part of the process that requires energy is the final purification of the alcohol, which was not possible to estimate it from literature.

Hence, this information was used to create a model for the production of the alcohol using a process simulation software. With this approach, it was possible to quantify also the energy demand for the separation. Energy integration was used to consider the reuse of heat from the reaction steps into separation units, since this is a common practice in chemical plants. The heat needed for the separation was entirely covered by the heat released in the reaction. Excess heat may be used in other parts of the plant, but no benefit from this energy were credited to the ethylhexanol production to be more conservative. The cooling was assumed to be done with water at 20 °C in a closed loop. A net consumption of 5% of the circulating water was considered due to evaporation and losses.

The quantity of reactants required per kg of 2-ethylhexanol was estimated using stoichiometry of the reaction. A complete conversion of the butyraldehyde has been assumed. The amount of sodium hydroxide to be replaced after step 2 is calculated considering a 2% concentration in the aqueous phase (Bahrmann et al., 2013).

The hydrogenation step is assumed to happen without losses of reagents and product due to lack of information. The consumption hydrogenation catalyst is considered a cut-off.

Table A 27 shows the inputs and output of the unit process describing the production of 2-ethylhexanol.

Table A 27. Life cycle inventory for the production of 1 kg of 2-ethyl hexanol

Inventory data		**Quantity**	**Unit**	**Dataset**
Input	Carbon monoxide	430	g	Carbon monoxide {RER}| production | APOS, U
	Hydrogen	62	g	Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation | APOS, U
	Propylene	64.6	g	Propylene {RER}| production | APOS, U
	Sodium hydroxide	2.75	g	Sodium hydroxide, without water, in 50% solution state {RER}| chlor-alkali electrolysis, membrane cell | APOS, U
	Heat	0	MJ	Heat, district or industrial, natural gas {RER}| market group for | APOS, U
	Electricity	0.182	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
Output	Wastewater to treatment	0.138	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

Acetyl tributyl citrate (ATBC)

The modelling of the plasticiser production has been developed using the stoichiometry to calculate the amount of each reagent. The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method were applied. Table A 28 summarises the amount of raw materials and transport required for the raw materials acquisition stage. Table A 29 shows the inventory data regarding the manufacturing of the plasticiser. Since no reliable data regarding the energy input for the ATBC manufacturing were found in literature, a process simulation software was used to estimate the energy flows. Below the syntheses of acetic anhydride, citric acid and butanol are briefly described.

Table A 28. Life cycle inventory for the raw materials required for 1 kg of ATBC

Inventory data		**Quantity**	**Unit**	**Dataset**
Raw materials	Acetic Anhydride	0.254	kg	Acetic anhydride {RER}| production, ketene route | APOS, U
	Citric Acid	0.477	kg	Citric acid {RER}| production | APOS, U
	Butanol	0.552	kg	1-butanol {RER}| hydroformylation of propylene | APOS, U
Transport	Ship	0.347	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.308	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.167	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table A 29. Life cycle inventory for the manufacturing of 1 kg of ATBC

Inventory data		**Quantity**	**Unit**	**Dataset**
Input	Heat	0.462	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Cooling water	0.0048	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Output	Wastewater to WWTP	0.283	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

Synthesis of acetic anhydride

The production process of acetic anhydride consists of two stages. Acetone is converted to methane and ketene, through its cracking at high temperature and pressure. The methane formed from this reaction is then burnt to provide part of the energy required by the process, while the other product, ketene, it further reacts with acetic acid to produce acetic anhydride (Held et al., 2000).

Synthesis of citric acid

Citric acid is produced by a fermentation process which employs a strain of the micro-organism *Aspergillus niger* to convert sugars into citric acid. The dataset Citric acid {RER}| production | APOS, U from Ecoinvent was used to model it.

Synthesis of butanol

1-butanol (also called n-butanol) is industrially produced mainly by propylene hydroformylation or from coal through a Fischer-Tropsch process (Sutter, 2007). For this study, it has been assumed that all the butanol is produced with the hydroformylation process.

The production of the precursors, citric acid, n-butanol and acetic anhydride, are modelled with secondary data from ecoinvent shown in Table A 28.

Di(2-ethyl hexyl) Adipate – DEHA

DEHA is one of the esters derived from adipic acid. It is used in a broad spectrum of application, from food packaging to construction sector. Its production is based on acid-catalysed esterification of adipic acid with 2-ethyl hexanol as described in Section 2.1.2

Primary data for the synthesis of the plasticisers were not available, therefore data from the ecoprofile (ECPI, 2015) of DINP were used as proxy for the DEHA due to the similarity in the esterification reaction. The amount of catalyst consumed per unit of product is considered in the cut-off.

The modelling of the plasticiser production has been developed using the stoichiometry to calculate the amount of adipic acid and 2-ethylhexanol needed. The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. Table A 30 summarise the quantity of raw materials and transport required for the plasticiser manufacturing. The inputs and outputs to the manufacturing stage are modelled according to the DINP Ecoprofile (ECPI, 2015), and they are summarised in Table A 31.

Table A 30. Life cycle inventory for the raw material required for 1 kg of DEHA

Inventory data		Quantity	Unit	Dataset
Raw materials	Adipic Acid	0.394	kg	Adipic acid {RER}| production | APOS, U
	2-ethylhexanol	0.703	kg	See Table A 27
Transport	Ship	0.296	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.263	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.143	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table A 31. Life cycle inventory for the manufacturing of 1 kg of DEHA

Inventory data		Quantity	Unit	Dataset
Input	Heat	0.97	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
	Deionised water	0.14	kg	Water, deionised {Europe without Switzerland}| market for water, deionised | APOS, U
	Cooling water	8.8	l	Water, cooling, unspecified natural origin, Europe without Switzerland
	Process water	0.004	kg	Water, cooling, unspecified natural origin, Europe without Switzerland
Output	Wastewater to WWTP	0.15	kg	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U
	Water from cooling	8.5	kg	Water, Europe without Switzerland
	Water vapour	0.35	kg	-

Synthesis of Adipic Acid

Adipic acid, a linear dicarboxylic acid, it is a fundamental chemical building block for the synthesis of a wide range of molecules (Skoog et al., 2018): about the 65% of its worldwide production is applied to produce nylon-6,6-polyamide (Deng Mao, 2015); it is also used to produce polyurethanes, paints, coatings, plasticisers and as food additive (Polen et al., 2013). Its production process is based on the acid oxidation with nitric acid of a mixture of cyclohexanol and cyclohexanone, which is obtained by oxidation of cyclohexane. The production of adipic acid is modelled with secondary data from Ecoinvent, while the supply chain of the ethyl hexanol is modelled as reported in Table A 27.

Di(2-ethyl hexyl) Terephthalate – DEHT

The modelling of the plasticiser production has been developed using the stoichiometry to calculate the amount of terephthalic acid and 2-ethylhexanol. The catalyst used to promote the esterification is included in the cut-off. The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. Table A 32 summarise the quantity of raw materials and transport required for the raw material acquisition stage. The input and output flows are the same shown in Table A 31 for the manufacturing of DEHA.

Table A 32. Life cycle inventory for the raw material required for 1 kg of DEHT

Inventory data		Quantity	Unit	Dataset
Raw materials	2-Ethylhexanol	0.667	kg	See Table A 27
	Terephthalic acid	0.425	kg	Purified terephthalic acid {RER}| production | APOS, U
Transport	Ship	0.295	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.262	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.142	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Synthesis of terephthalic acid

Terephthalic acid is one of the most relevant intermediate chemicals globally. This is due mainly to its use for the synthesis of polyethylene terephthalate (PET). The industrial production is done almost completely with the Amoco process, which is fed with p-xylene from BTX fractionation and oxygen. Due to the high purity required for PET production, which is the main use of terephthalic acid, the production is coupled with a purification process consisting in the hydrogenation of impurities and subsequent distillation to eliminate a small amount of unreacted p-xylene and other by-products which affects the colour of the final product (Sheehan, 2011).

The production of terephthalic acid is modelled with secondary data from ecoinvent, while the supply chain of the ethylhexanol is modelled as shown in Table A 27.

Di-isononyl cyclohexanoate – DINCH

Cyclohexanoates are plasticisers derived from the phthalates through the hydrogenation of the aromatic ring. Their similarity in the chemical structure allows for an easy replacement of the phthalates reducing the safety concerns. DINCH is one of the most common cyclohexanoates and it is the result of the catalytic hydrogenation of DINP as described in Section 2.1.2

The unit process for the raw material acquisition of the plasticiser is created using secondary data for the precursors (DINP and hydrogen). The raw materials are assumed to be sourced in Europe, therefore the average distances described in the PEF method have been assumed. The quantity of the raw materials and transport required for the plasticiser manufacturing are summarised in Table A 33. The inputs and outputs required for the hydrogenation process is unknown, hence proxy data were extracted from the hydrogenation of benzene to cyclohexane using the ecoinvent dataset *Cyclohexane {RER}| production | APOS, U*. Table A 34 shows a summary of the unit process inputs and outputs.

Table A 33. Life cycle inventory for the raw materials required for 1 kg of DINCH

Inventory data		Quantity	Unit	Dataset
Raw materials	DINP	0.986	kg	Dataset derived from DINP Ecoprofile
	Hydrogen	0.014	kg	Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation | APOS, U
Transport	Ship	0.270	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.240	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.130	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table A 34. Life cycle inventory for the manufacturing of 1 kg of DINCH

Inventory data		Quantity	Unit	Dataset
Input	Heat	2.82	MJ	Heat, district or industrial, natural gas {RER}| market group for | APOS, U
	Heat	1.57	MJ	Heat, district or industrial, other than natural gas {RER}| market group for | APOS, U
	Electricity	0.127	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
	Catalyst	0.03	g	Nickel 99.5% {GLO}| market for | APOS
	Water deionised	0.003	kg	Water deionised {CH}| market for water
	Water deionised	0.947	kg	Water deionised {Europe without Switzerland}| market for water
	Water, cooling	0.008	m^3	Water, cooling, unspecified natural origin, RER
Output	Evaporated water	0.0033	m^3	Water
	Discharged water	0.0057	m^3	Water, Europe without Switzerland

Epoxidised soybean oil - ESBO

The production of the precursors, soybean oil, and hydrogen peroxide is modelled using secondary data from Ecoinvent. The formic acid and the sulphuric acid used are considered in the cut-off, since they behave like catalyst in the reaction. Table A 35 summarises the quantity of raw materials and transport required for the plasticiser manufacturing. A brief description of the production route of the raw materials is provided below.

The energy requirements in the epoxidation process, the net water consumed and the amount of waste produced were derived from the information disclosed in an Environmental Product Declaration for the ESBO (Hairma (Nantong) Technology, 2022) and are reported in Table A 36.

Table A 35. Life cycle inventory for the raw material required for 1 kg of ESBO.

Inventory data		Quantity	Unit	Dataset
Raw materials	Soybean Oil	0.902	kg	Soybean oil, crude {RER}| soybean meal and crude oil production | APOS, U
	Hydrogen peroxide	0.209	kg	Hydrogen peroxide, without water, in 50% solution state {RER}| market for hydrogen peroxide, without water, in 50% solution state | APOS, U
Transport	Ship	0.300	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.267	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.144	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Table A 36. Unit process for the manufacturing for 1 kg of ESBO.

Inventory data		Quantity	Unit	Dataset
Input	Electricity	0.0371	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
	Steam	0.143	kg	Steam, in chemical industry {RER}| production | APOS, U
	Water	0.0002	kg	Water, river, Europe without Switzerland
Output	Hazardous waste	0.0013	kg	Refinery sludge {Europe without Switzerland}| treatment of refinery sludge, hazardous waste incineration | APOS, U

Extraction of soy oil

In the mechanical extraction soybeans are cracked and squeezed to produce the oil. In the case of solvent extraction, after the crushing step, the oil is extracted with a solvent such as hexane (Riaz, 2005) to maximise the yield.

Synthesis of Hydrogen Peroxide

The most common process for the production of hydrogen peroxide is the auto-oxidation (AO) or anthraquinone process, which is the most relevant industrial process. In a first step, hydrogen peroxide is produced by reducing alkyl-anthraquinone with hydrogen in the presence of a catalyst to the hydroquinone. Then the catalyst is removed and the hydroquinone is oxidised – usually with air – back to the quinone and in the same time hydrogen peroxide is produced (Althaus et al., 2007; Boustead Fawer, 1998).

PVC and additives

For the modelling of the PVC that is blended with the plasticiser, a secondary dataset representative of emulsion PVC, since this is the polymer commonly used for the plastisol applications. Other additives are also modelled using secondary datasets from Ecoinvent as shown in Table A 37. This limitation is due to data availability but it is acceptable considering that the purpose of the study is to evaluate differences in impacts of different plasticisers.

Since no secondary dataset for zinc stearate production is available, a customized dataset was created with literature data. Zinc stearate production involves zinc oxide and stearic acid at 140 °C and under atmospheric pressure (Gönen et al., 2005), Table A 37 shows the inputs and output calculated using stoichiometry calculations, Energy consumption for heating or cooling is considered a cut-off.

Table A 37. Life cycle inventory for the production of 1 kg of Zinc Stearate

Inventory data		Quantity	Unit	Dataset
Input	Zinc Oxide	128.8	g	Zinc oxide {RER}| production | APOS, U
	Stearic Acid	899.8	g	Stearic acid {GLO}| stearic acid production | APOS, U
Output	Water	0.0285	l	Wastewater, average {Europe without Switzerland}| treatment of wastewater, average, capacity 1E9l/year | APOS, U

A7.2 Compounding and manufacturing of the gasket

This section reports the modelling and inventory for the production of the gasket. This includes the production of the plastisol and the production of the gasket that is applied inside the metal lid. These two processes are often done in the same plant, since the metal cap producer is usually producing its own plastisol, hence no transport between the two processes was considered.

Compounding: Plastisol Production

The inventories of plastisol production for each plasticiser are reported Table A 38. The composition reported in Table 3 is based on Bayer et al., 1988; Giessler Ratliff, 1968 works and confirmed by industry stakeholders.

Table A 38. List of the raw materials required for the manufacturing of the plastisol for each plasticiser and of their transport to the compounding facility

Data inventory		**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**	**Unit**	**Dataset**
Input	Plasticiser	358.2	371.7	341.7	365.0	378.2	394.0	g	See section 2.1.2.2
	E-PVC	477.6	467.5	489.8	472.5	462.6	456.7	g	Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation | APOS, U
	Blowing Agent (Sodium Bicarbonate)	5.73	5.6	5.9	5.7	5.6	5.21	g	Sodium bicarbonate {RER}| soda production, solvay process | APOS, U
	Stabiliser (Zinc Stearate)	11.94	11.7	12.2	11.8	11.6	10.85	g	See section Table A 37
	Lubricant (stearic acid)	40.59	39.7	41.6	40.2	39.3	36.90	g	Stearic acid {GLO}| stearic acid production | APOS, U
	Pigment (TiO_2)	5.731	5.6	5.9	5.7	5.6	5.210	g	Titanium dioxide {RER}| production, sulfate process | APOS, U
	Filler (calcium carbonate)	100.3	98.2	102.9	99.2	97.2	91.2	g	Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated | APOS, U
Transport	Ship	0.270	0.270	0.270	0.270	0.270	0.270	t*km	Transport, freight, inland waterways, barge tanker {RER}| market| APOS, U
	Train	0.240	0.240	0.240	0.240	0.240	0.240	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
	Truck	0.130	0.130	0.130	0.130	0.130	0.130	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

Below, Table A 39 shows the energy and utilities requirements for mixing and cooling the compound. The energy requirements were estimated from a previous work, in which a similar mixture was applied (Boluk et al., 1990), while the cooling water was calculated based on an experimental study (Nakajima, 2000) assuming a net loss of 5% in the industrial application. The amount of energy and cooling water consumption was assumed to be the same for all the six similar plasticiser mixtures.

Table A 39. Inventory data for the compounding of 1 kg of plastisol for all the plasticisers

Input	**Quantity**	**Unit**	**Dataset**
Electricity	0.917	kWh	Electricity, medium voltage {RER}| market group for | APOS, U
Cooling Water	0.0565	m^3	Water, cooling, unspecified natural origin, RER

Gasket manufacturing

Table A 40 shows the energy requirements for the steps described in this section.

Table A 40. Data inventory for 1 kg of manufactured gasket

Input	**Quantity**	**Unit**	**Dataset**
Heat in Pre-heating	0.108	MJ	Heat, from steam, in chemical industry {RER}| steam production, as energy carrier, in chemical industry | APOS, U
Electricity in Curing	0.883	kWh	Electricity, medium voltage {RER}| market group for | APOS, U

A7.3 Distribution

The distribution phase considers the transport of the cap (and hence the gasket) to the final customer, which is the company using it to can the food. In this case, the average transport for the packaging material is estimated from PEF method, and they are presented in Table A 41.

Table A 41. Transport distances for 1 kg of gasket

Means of transport	**Quantity**	**Unit**	**Dataset**
Ship	0.360	t*km	Transport, freight, inland waterways, barge {RER}| market| APOS, U
Train	0.280	t*km	Transport, freight train {Europe without Switzerland}| market for | APOS, U
Truck	0.230	t*km	Transport, freight, lorry >32 metric ton, euro4 {RoW}| market, EURO4 | APOS, U

A7.4 Use phase

The use phase of the gasket starts when the cap is used in the canning process. Any process involved in this phase is done to preserve the food, and therefore the environmental impact shall be accounted in the system boundaries of the food and excluded from this analysis. The final use of the gasket is linked to the use of the cap and its content, and it can be reasonably assumed to be a single use packaging.

A7.5 End-of-life

The share of waste caps sent to incineration or disposal has been assumed using the data of the average European municipal waste treatment (Eurostat, 2022), which is 53% to incineration and 47% to landfill. The disposal of the gasket is modelled specifically considering the composition of the gasket with the different plasticisers (see Table 3). Then, for each plasticiser a unit process for the incineration and one for the sanitary landfill have been developed, which represent the specific emissions due to either the incineration or landfill of each plasticiser. This was done using the model developed in Doka, (2020), fed with the elementary composition of the plasticisers (see Table A 42). Then, the plasticiser specific dataset was coupled with the equivalent dataset for the disposal of PVC from Ecoinvent and with the one developed for the disposal of the added stabilisers.

Finally, the end-of-life of the whole gasket is modelled as shown in Figure A 4 considering the share of gasket made with the different materials (PVC, plasticiser and additives) and the share of treatment. A summary of the life cycle inventory per each type of gasket is provided in Table A 43, Table A 44 and Table A 45 showing the inputs and outputs of the customized dataset developed for the incineration and landfill respectively.

Table A 42. Elementary composition of plasticisers and additives used to calculate specific disposal emissions

Elementary composition	**DEHP [%]**	**ATBC [%]**	**DEHA [%]**	**DEHT [%]**	**DINCH [%]**	**ESBO [%]**	**Additives [%]**
C	73.8	59.7	71.3	73.8	74.2	70.2	33.0
H	9.8	8.5	11.4	9.8	10.5	10.1	4.3
O	16.4	31.8	17.3	16.4	15.2	19.7	35.3
Na	0	0	0	0	0	0	0.8
Ca	0	0	0	0	0	0	24.8
Zn	0	0	0	0	0	0	0.9
Ti	0	0	0	0	0	0	1.7
% of biogenic C	0	30	0	0	0	100	34

Figure A 4. Model of waste management of the gasket, considering the share of incineration and landfill and the specific composition of each gasket.

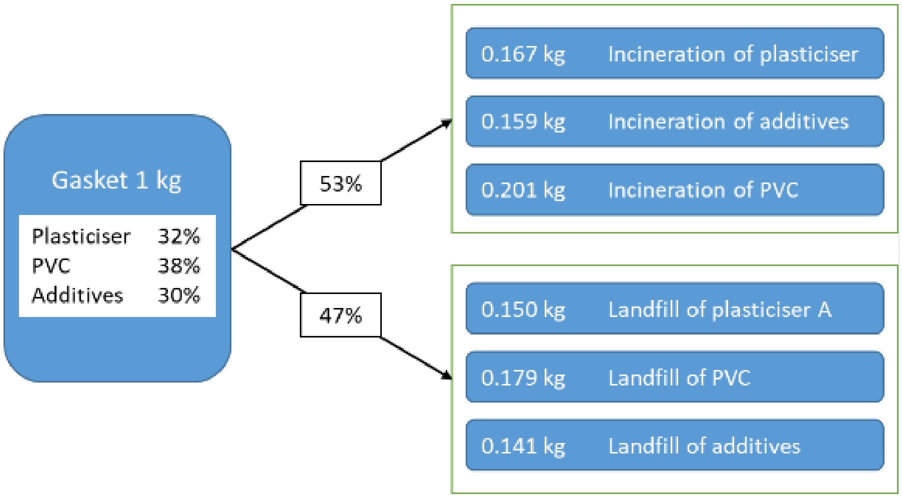


Table A 43. Share of the waste management of 1 kg of gasket for each of the considered plasticisers, based on the average European municipal waste treatment and the composition of each plasticisers, and datasets associated to each waste treatment

Input	**DEHP**	**ATBC**	**DEHA**	**DEHT**	**DINCH**	**ESBO**	**Unit**	**Dataset**
Incineration of plasticiser	0.190	0.197	0.181	0.193	0.200	0.201	kg	Custom dataset (see Table A 44)
Incineration of the PVC	0.253	0.248	0.260	0.250	0.245	0.244	kg	Waste polyvinylchloride {CH}| treatment of, municipal incineration | APOS, U
Incineration of additives	0.087	0.085	0.089	0.086	0.084	0.084	kg	Custom dataset (see Table A 44)
Landfill of plasticiser	0.168	0.175	0.161	0.172	0.178	0.179	kg	Custom dataset (see Table A 45)
Landfill of the PVC	0.225	0.220	0.230	0.222	0.217	0.217	kg	Waste polyvinylchloride {CH}| treatment of, sanitary landfill | APOS, U
Landfill of additives	0.077	0.076	0.079	0.076	0.075	0.075	kg	Custom dataset (see Table A 45)

Table A 44. Life cycle inventory of the incineration of 1 kg of gasket for each plasticiser and for 1 kg of additives, modelled according to (Doka, 2020)

	Unit	DEHP	ATBC	DEHA	DINCH	DEHT	ESBO	Additives	Dataset
Input from technosphere									
Metalliferous hydroxide sludge	kg	4.6E-04	3.7E-04	4.5E-04	4.6E-04	4.6E-04	4.4E-04	2.2E-02	Metalliferous hydroxide sludge {GLO}| market for metalliferous hydroxide sludge | APOS, U
Sodium hydroxide, without water, in 50% solution	kg	2.5E-05	2.0E-05	2.4E-05	2.5E-05	2.5E-05	2.4E-05	1.2E-03	Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U
Hydrochloric acid, without water, in 30% solution	kg	3.9E-05	3.1E-05	3.7E-05	3.9E-05	3.9E-05	3.7E-05	1.6E-03	Hydrochloric acid, without water, in 30% solution state {RER}| market for | APOS, U
Inorganic chemicals	kg	1.8E-05	1.4E-05	1.7E-05	1.8E-05	1.8E-05	1.7E-05	1.1E-04	Chemical, inorganic {GLO}| market for chemicals, inorganic | APOS, U
Cement	kg	7.2E-04	5.8E-04	6.9E-04	7.2E-04	7.2E-04	6.8E-04	2.3E-02	Cement, unspecified {CH}| market for cement, unspecified | APOS, U
Waste cement, hydrated	kg	1.8E-03	1.5E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	5.8E-02	Waste cement, hydrated {CH}| market for waste cement, hydrated | APOS, U
Transport, freight, lorry	t*km	6.5E-04	5.6E-04	6.3E-04	6.5E-04	6.5E-04	6.2E-04	1.9E-02	Transport, freight, lorry 16-32 metric ton, EURO4 {RER}| transport, freight, lorry 16-32 metric ton, EURO4 | APOS, U
Ammonia, liquid	kg	8.3E-04	6.3E-04	8.5E-04	8.6E-04	8.3E-04	8.0E-04	3.15E-04	Ammonia, liquid {RER}| market for | APOS, U
Heat, district or industrial, natural gas	MJ	1.6E-01	1.2E-01	1.6E-01	1.6E-01	1.6E-01	1.5E-01	5.9E-02	Heat, district or industrial, natural gas {CH}| market for heat, district or industrial, natural gas | APOS, U
Titanium dioxide	kg	5.2E-05	3.9E-05	5.3E-05	5.4E-05	5.2E-05	5.0E-05	2.0E-04	Titanium dioxide {RER}| market for | APOS, U
Chromium oxide, flakes	kg	1.1E-06	8.0E-07	1.1E-06	1.1E-06	1.1E-06	1.0E-06	4.03E-07	Chromium oxide, flakes {GLO}| market for | APOS, U
Hydrogen peroxide, without water, 50% solution	kg	8.7E-05	7.0E-05	8.4E-05	8.7E-05	8.7E-05	8.3E-05	4.1E-03	Hydrogen peroxide, without water, in 50% solution state {RER}| market for hydrogen peroxide, without water, in 50% solution state | APOS, U
Spent activated carbon with mercury	kg	1.8E-05	1.4E-05	1.7E-05	1.8E-05	1.8E-05	1.7E-05	1.1E-04	Spent activated carbon with mercury {GLO}| market for | APOS, U
Water, decarbonised	kg	2.1E-01	1.7E-01	2.0E-01	2.1E-01	2.1E-01	2.0E-01	1.3E+00	Water, decarbonised {CH}| water production, decarbonised | APOS, U

	Unit	DEHP	ATBC	DEHA	DINCH	DEHT	ESBO	Additives	Dataset
Input from technosphere									
Municipal waste incineration facility	unit	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	2.5E-10	Municipal waste incineration facility {CH}| construction | APOS, U
Slag landfill	unit	2.4E-11	2.1E-11	2.4E-11	2.4E-11	2.4E-11	2.4E-11	7.1E-10	Slag landfill {CH}| construction | APOS, U
Process-specific burdens, slag landfill	kg	1.4E-02	1.2E-02	1.3E-02	1.4E-02	1.4E-02	1.3E-02	4.0E-01	Process-specific burdens, slag landfill {CH}| processing | APOS, U
Residual material landfill	unit	3.7E-12	3.0E-12	3.6E-12	3.8E-12	3.7E-12	3.6E-12	1.2E-10	Residual material landfill {CH}| construction | APOS, U
Process-specific burdens, residual material landfill	kg	1.8E-03	1.5E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	5.7E-02	Process-specific burdens, residual material landfill {CH}| processing | APOS, U
Input from nature									
Oxygen, from air	kg	5.2E+00	3.9E+00	5.3E+00	5.3E+00	5.2E+00	5.0E+00	1.96E+00	
Emissions to air									
Carbon monoxide, fossil	kg	2.4E-05	1.1E-05	2.2E-05	2.2E-05	2.4E-05		4.9E-05	
Carbon monoxide, biogenic	kg		2.7E-05				2.6E-05	1.3E-05	
Carbon dioxide, fossil	kg	2.7E+00	6.5E-01	2.6E+00	2.7E+00	2.7E+00		9.5E-01	
Carbon dioxide, biogenic	kg		1.5E+00				2.6E+00	2.5E-01	
Methane, fossil	kg	2.1E-07	1.0E-07	1.9E-07	1.9E-07	2.1E-07		4.3E-07	
Methane, biogenic	kg		2.4E-07				2.3E-07	1.1E-07	
Nitrogen oxides	kg	3.1E-04	2.3E-04	3.2E-04	3.2E-04	3.1E-04	3.0E-04	1.17E-03	
Ammonia	kg	9.8E-07	7.4E-07	1.0E-06	1.0E-06	9.8E-07	9.4E-07	3.7E-07	
NMVOC, non-methane volatile organic compounds	kg	6.3E-07	1.0E-06	5.9E-07	5.8E-07	6.3E-07	6.9E-07	1.65E-06	
Particulates, < 2.5 um	kg	1.7E-06	2.7E-06	1.5E-06	1.5E-06	1.7E-06	1.8E-06	4.3E-06	
Particulates, > 2.5 um, and < 10um	kg	8.3E-09	1.3E-08	7.8E-09	7.6E-09	8.3E-09	9.1E-09	2.2E-08	

	Unit	DEHP	ATBC	DEHA	DINCH	DEHT	ESBO	Additives	Dataset
Input from technosphere									
Dioxins, measured as 2,3,7,8-tetrachlorodibenzo-p-dioxin	kg	2.8E-14	4.5E-14	2.6E-14	2.5E-14	2.8E-14	3.0E-14	7.2E-14	
Benzene	kg	1.4E-08	2.2E-08	1.3E-08	1.3E-08	1.4E-08	1.5E-08	3.6E-08	
Toluene	kg	2.8E-08	4.5E-08	2.6E-08	2.5E-08	2.8E-08	3.0E-08	7.2E-08	
Benzene, pentachloro-	kg	7.3E-11	1.2E-10	6.8E-11	6.7E-11	7.3E-11	8.0E-11	2.0E-10	
Benzene, hexachloro-	kg	2.9E-11	4.7E-11	2.7E-11	2.7E-11	2.9E-11	3.2E-11	7.6E-11	
Phenol, pentachloro-	kg	6.0E-12	9.8E-12	5.6E-12	5.5E-12	6.0E-12	6.6E-12	1.6E-11	
Benzo(a)pyrene	kg	3.1E-13	5.0E-13	2.9E-13	2.8E-13	3.1E-13	3.4E-13	8.1E-13	
Water	m^3	9.2E-04	7.9E-04	1.0E-03	9.8E-04	9.2E-04	9.4E-04	1.1E-03	
Emissions to water									
Water	m^3	7.1E-05	5.7E-05	6.9E-05	7.2E-05	7.1E-05	6.8E-05	4.2E-03	
BOD5, Biological Oxygen Demand	kg	5.5E-04	4.4E-04	5.3E-04	5.5E-04	5.5E-04	5.2E-04	2.5E-04	
COD, Chemical Oxygen Demand	kg	5.6E-04	4.5E-04	5.4E-04	5.6E-04	5.6E-04	5.3E-04	2.5E-04	
TOC, Total Organic Carbon	kg	2.4E-04	2.0E-04	2.4E-04	2.5E-04	2.4E-04	2.3E-04	1.1E-04	
DOC, Dissolved Organic Carbon	kg	2.4E-04	2.0E-04	2.4E-04	2.5E-04	2.4E-04	2.3E-04	1.1E-04	
BOD5, Biological Oxygen Demand, long-term	kg	1.8E-03	1.4E-03	1.7E-03	1.8E-03	1.8E-03	1.7E-03	2.5E-04	
COD, Chemical Oxygen Demand, long-term	kg	5.5E-03	4.4E-03	5.3E-03	5.5E-03	5.5E-03	5.2E-03	2.5E-04	
TOC, Total Organic Carbon, long-term	kg	2.2E-03	1.8E-03	2.1E-03	2.2E-03	2.2E-03	2.1E-03	1.1E-04	
DOC, Dissolved Organic Carbon, long-term	kg	2.2E-03	1.8E-03	2.1E-03	2.2E-03	2.2E-03	2.1E-03	1.1E-04	

Table A 45. Life Cycle Inventory of the landfill of 1 kg of gasket for each of the plasticiser and for 1 kg of additives, modelled according to (Doka, 2020).

	Unit	**DEHP**	**ATBC**	**DEHA**	**DINP**	**DINCH**	**DEHT**	**ESBO**	**Additives**	**Dataset**
Input from technosphere										
Transport, freight, lorry	t*km	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	7.74E-07	Transport, freight, lorry >32 metric ton, EURO4 {RER}| transport, freight, lorry >32 metric ton, EURO4 | APOS, U
Heat, district or industrial, natural gas	MJ	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	4.67E-05	Heat, district or industrial, natural gas {RER}| market group for | APOS, U
Electricity, low voltage	kWh	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	8.49E-05	Electricity, low voltage {RER}| market group for | APOS, U
Heat, district or industrial, other than natural gas	MJ	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	1.64E-03	Heat, district or industrial, other than natural gas {Europe without Switzerland}| market for heat, district or industrial, other than natural gas | APOS, U
excavation, hydraulic digger	m^3	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Excavation, hydraulic digger {RER}| processing | APOS, U
excavation, skid-steer loader	m^3	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Excavation, skid-steer loader {RER}| processing | APOS, U
diesel, burned in building machine	MJ	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	4.84E-02	Diesel, burned in building machine {GLO}| market for | APOS, U
gravel, round	kg	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	1.60E-01	Gravel, round {CH}| gravel and sand quarry operation | APOS, U
tap water	kg	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	3.88E-04	Tap water {Europe without Switzerland}| tap water production, conventional with biological treatment | APOS, U
Input from nature										
Occupation, construction site	m^2*y	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	
Occupation, dump site	m^2*y	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	1.5E-03	

	Unit	DEHP	ATBC	DEHA	DINP	DINCH	DEHT	ESBO	Additives	Dataset
Occupation, shrub land, sclerophyllous	m^2*y	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	2.5E-04	
Occupation, traffic area, road network	m^2*y	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	1.9E-03	
Transformation, from pasture, man made	m^2	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	6.0E-05	
Transformation, from dump site, sanitary landfill	m^2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, from shrub land, sclerophyllous	m^2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to dump site, sanitary landfill	m^2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to shrub land, sclerophyllous	m^2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to forest, unspecified	m^2	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	5.0E-05	
Transformation, to traffic area, road network	m^2	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	
Emissions to water										
BOD5, Biological Oxygen Demand, long term	kg	0.191	0.155	0.185	0.193	0.192	0.191	0.182	0.273	
COD, Chemical Oxygen Demand, long term	kg	0.807	0.653	0.780	0.816	0.812	0.807	0.768	1.151	
TOC, Total Organic Carbon, long term	kg	0.738	0.597	0.713	0.746	0.742	0.738	0.702	1.053	
DOC, Dissolved Organic Carbon	kg	0.738	0.597	0.713	0.746	0.742	0.738	0.702	1.053	

Annex 8. Step 4 - Detailed results on Environmental sustainability assessment

Following the PEF method, the potential environmental impacts are presented at the midpoint characterisation level for the life cycle of each of the six different plasticized gaskets and reported in Figure 17. Then, the characterised results are normalised using the factors recommended by the PEF. The normalised results are dimensionless and they represent the impact that is attributed to the chemical or material assessed compared to the total impact per person at a global scale. The normalised results are shown in Figure A 5.

From this comparison, for almost all the impact categories, the DEHT and DINCH gaskets result the one with the lowest impact in most of the categories. On the other hand, DEHA and ATBC show the highest value with and without normalization.

The PEF method includes a set of n weighing factors developed with the contribution of domain experts as well as reflecting panel based elicitations, aiming to reflect the relevance and the scientific robustness of the different impact categories (Sala et al., 2018) and these results are presented in Figure A 6. The set of normalization and weighing factors are presented in Annex 9.

Figure 17 do not provide the contribution of each sub-category to the Climate Change (i.e. from fossil, biogenic and land use/land transformation GHG emissions), but they are available in Table A 47. At the same time, for readability of the document, the characterized impacts in each life cycle stage are reported partially in interpretation section.

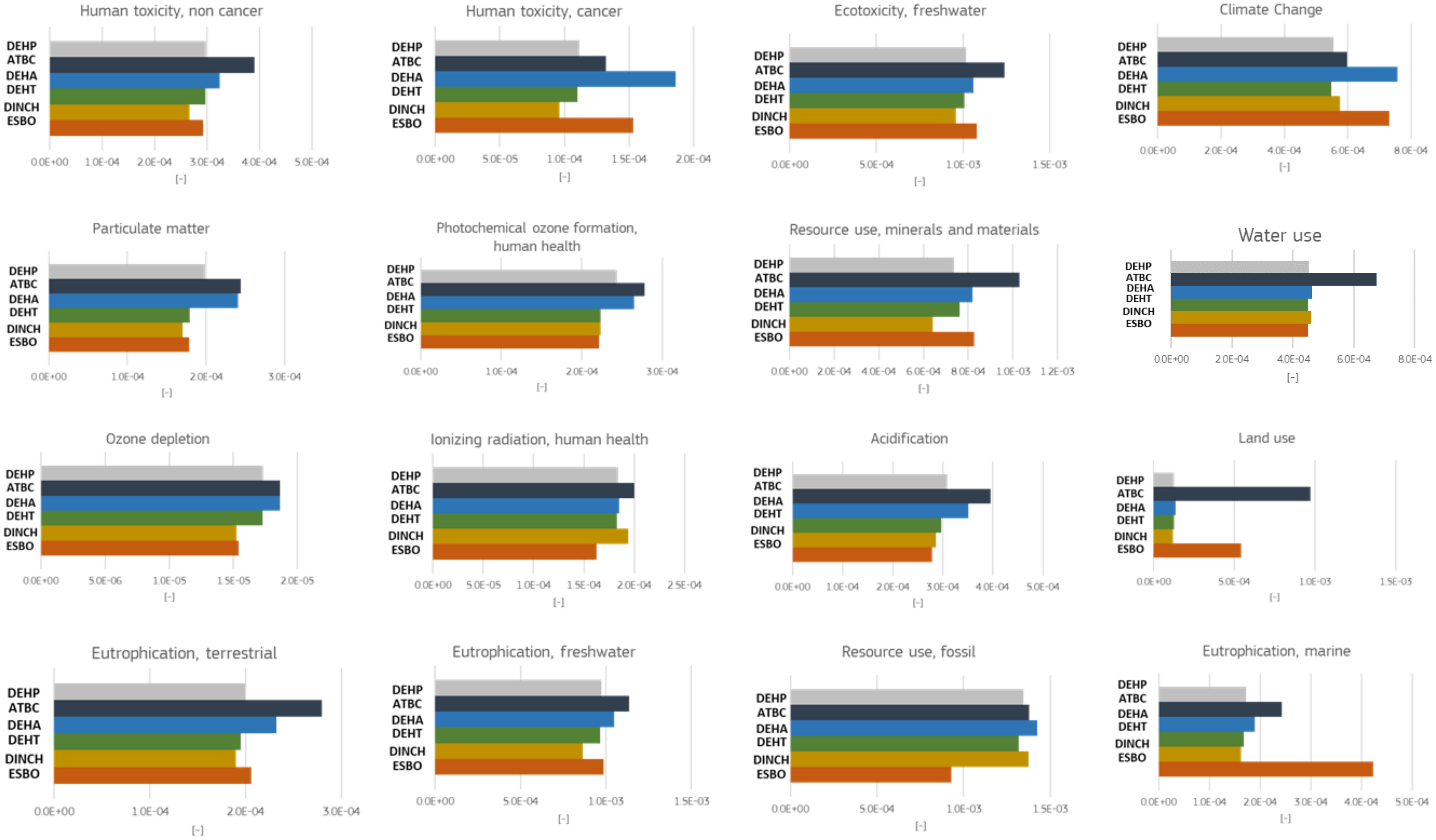
The results across the 16 impact categories show two different patterns. Some impact categories do not show significant differences among the plasticisers, such as the “Ionizing radiation, human health” and “Ecotoxicity, freshwater”, while others show significant differences among them, such as the “resource use, fossils” and the “land use”. Similarities and differences can be attributed mostly to the type and quantity of the plasticiser. The quantity of PVC and the additives change according to the plasticiser. In most cases, the precursors are petrochemicals, except for the ESBO and partly for the ATBC that are bio-based (i.e. the soy oil and the citric acid, respectively). This is reflected, for example, in the “land use” impact category for ATBC and ESBO which is higher than for all the other plasticisers due their precursors, while ESBO scores lower than the others on the “resource use, fossil”. Regarding the climate change indicator, DEHA shows the highest results, due to the higher impact of the adipic acid, followed by ESBO due to the emissions linked to land use change in soy oil production.

Moreover, it is important to recall that the toxicity-related impact categories, only measure the residual toxicity across the life cycle. They do not give any information on acute toxicity, for example the one linked to consumer exposure to the plasticisers. So, to have a more comprehensive picture of the toxicity aspects all the information from the steps 1 to 4 of the framework should be considered.

Finally, it has to be noted that a specific assessment of the significance of results and their related uncertainty has not been conducted at this stage, since the goal of the study was to test the applicability of the SSbD framework.

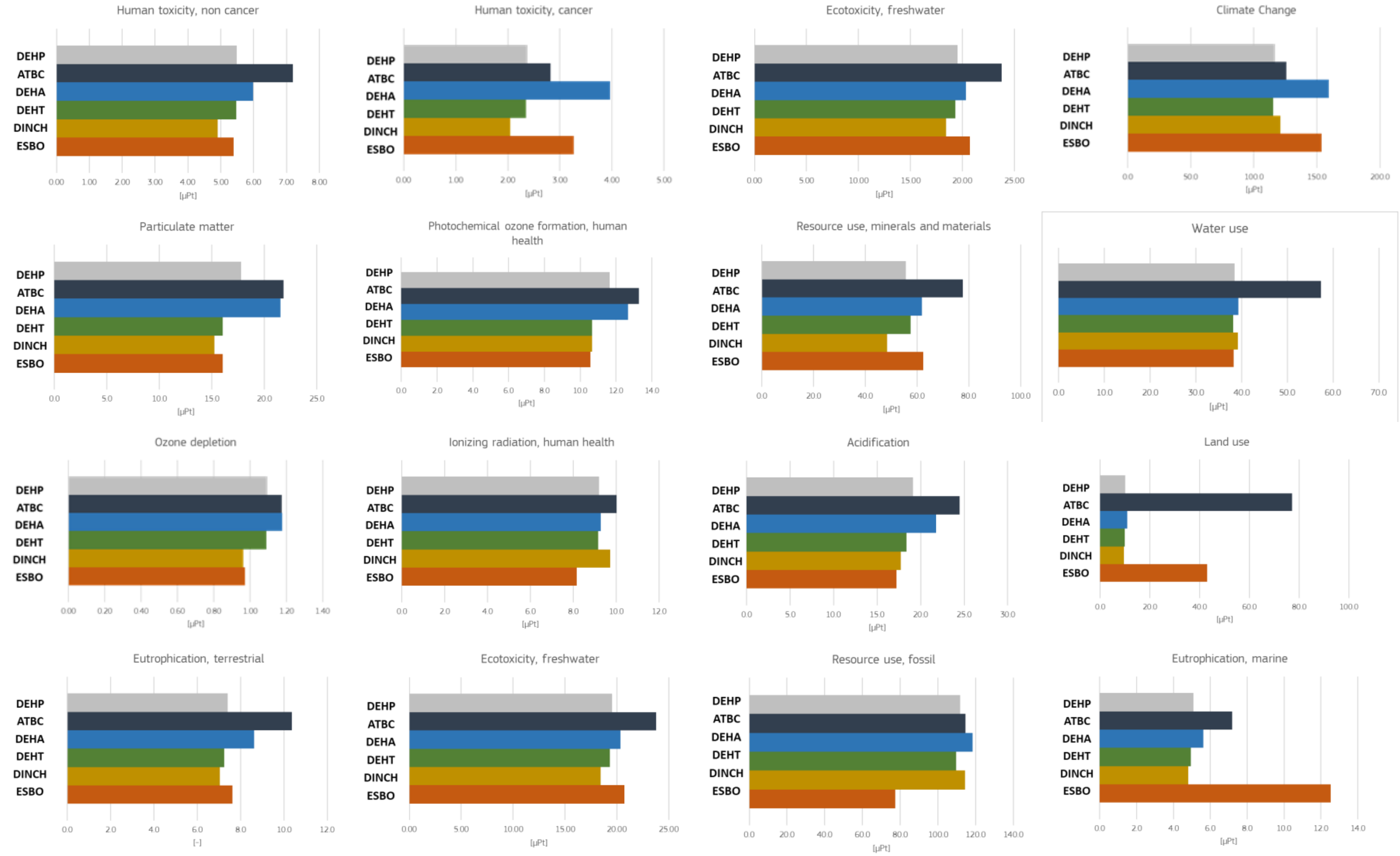
A8.1 Normalized results

Figure A 5. Cradle to grave normalized results for all the PEF impact categories and the six gaskets



A8.2 Weighted results

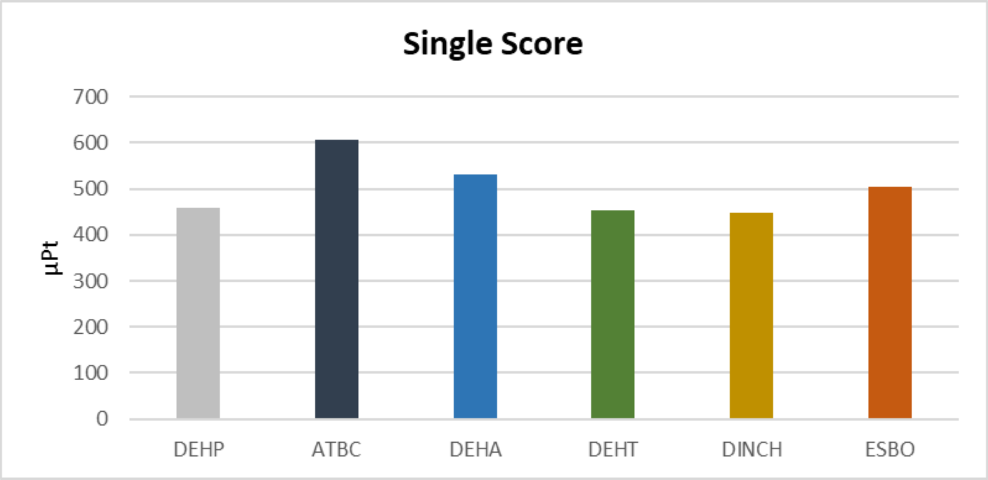
Figure A 6. Cradle to grave weighted results in micropoints (µPt) for all the EF impact categories and the six gaskets



A8.3 Single score

Figure A 7 presents the weighted values summed in a single score for each gasket. Among the six gaskets DEHT scores the lowest value, and it is also the only one that shows a reduction of impact compared with the phthalate one DEHP, which is the reference and it is indicated in grey colour. The single score does not show a plasticiser performing remarkably better than the others. However, taking into consideration the high concerns of the DEHP in terms of safety, the results show that DEHT could be the potential alternative solution performing better in terms of safety but still guarantying similar performances in terms of environmental sustainability without worsening this aspect. It is also important to notice that the weighting score of the PEF is one of the possible ways to aggregate different LCA indicators. This analysis will be used to make further considerations when a specific procedure for the SSbD scoring system will be established.

Figure A 7. Cradle to grave single weighted score results in micropoints (µPt) for the six gaskets. Starting from the reference (i.e. DEHP), DEHT is the only alternative performing slightly better. DEHA, DINCH and ESBO slightly worsen the environmental performance, while ATBC performs significantly worse than the reference.



A8.4 Interpretation of the LCA results

In the interpretation of the case study results, most relevant impact categories and life cycle stages of the studied systems are firstly identified in the following subsections.

Most relevant processes identified are reported in section A8.4.3 Identification of most relevant processes. The identification of most relevant elementary flows has been performed for climate change in this version of the report (see Annex 8).

The impacts of the End-of-life scenarios are presented below.

A8.4.1 Identification of most relevant impact categories

Table A 46 shows the most relevant impact categories identified for each gaskets (grey cells) based on normalised (Figure A 5) and weighted impacts (Figure A 6), according to the approach reported in EC (2021). Relevant categories were identified as those that cumulatively contribute to at least 80% of the total normalised and weighted impact of the considered impact categories. In particular, among the six gaskets the following relevant impact categories were identified in common as being those contributing the most: Climate Change, Resource use, fossil, Resource use, minerals and materials, Water use and Eutrophication, freshwater. These five categories were added to the analysis also Ecotoxicity, freshwater, which is relevant for all gaskets except DEHA; Acidification relevant only for DEHA; Land use that is relevant for ATBC and ESBO.

Table A 46. Cradle to grave weighting results (%) for the six gaskets. Impact categories with grey background represent 80% of the impacts.

Impact	ATBC	DEHA	DEHT	DINCH	ESBO
Climate change	20.7	30.1	25.5	27.0	30.4
Resource use, fossil	18.9	22.3	24.2	25.5	15.3
Resource use, minerals and metals	12.8	11.7	12.7	10.8	12.4
Water use	9.5	7.4	8.4	8.7	7.6
Eutrophication, freshwater	5.2	5.5	6.0	5.4	5.5
Ecotoxicity, freshwater	3.9	3.8	4.3	4.1	4.1
Acidification	4.0	4.1	4.1	4.0	3.4
Land use	12.7	2.1	2.2	2.1	8.5
Particulate matter	3.6	4.1	3.5	3.4	3.2
Photochemical ozone formation, human health	2.2	2.4	2.4	2.4	2.1
Ionizing radiation, human health	1.7	1.8	2.0	2.2	1.6
Eutrophication, terrestrial	1.7	1.6	1.6	1.6	1.5
Human toxicity, non-cancer	1.2	1.1	1.2	1.1	1.1
Eutrophication, marine	1.2	1.1	1.1	1.1	2.5
Human toxicity, cancer	0.5	0.7	0.5	0.5	0.7
Ozone depletion	0.2	0.2	0.2	0.2	0.2

The analysis might be then further elaborated, addressing contribution of individual elementary flows to the impact categories. For example, for climate change, it is possible to illustrate the results highlighting the contribution of individual type of drivers of climate change impacts.

Table A 47. Life cycle impacts on climate change for the six gaskets, split by sub-categories

Impact category	Unit	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Climate change, total	kg CO_2 eq	4.186	4.507	5.714	4.137	4.341	5.512
Climate change, fossil	kg CO_2 eq	4.153	4.469	5.680	4.104	4.310	3.170
Climate change, biogenic	kg CO_2 eq	0.019	0.021	0.020	0.019	0.018	0.021
Climate change, land use and land use change	kg CO_2 eq	0.014	0.018	0.014	0.014	0.013	2.321

Table A 48. Most relevant flows for climate change for each of the 6 gaskets

Elementary flow	DEHP	ATBC	DEHA	DEHT	DINCH	ESBO
Carbon dioxide, fossil	90%	89%	71%	90%	75%	51%
Methane, fossil	8%	7%	6%	7%	5%	4%
Dinitrogen monoxide	1%	2%	22%	1%	0%	3%
Carbon dioxide, land transformation	0%	0%	0%	0%	0%	42%

A8.4.2 Identification of most relevant Life Cycle stages

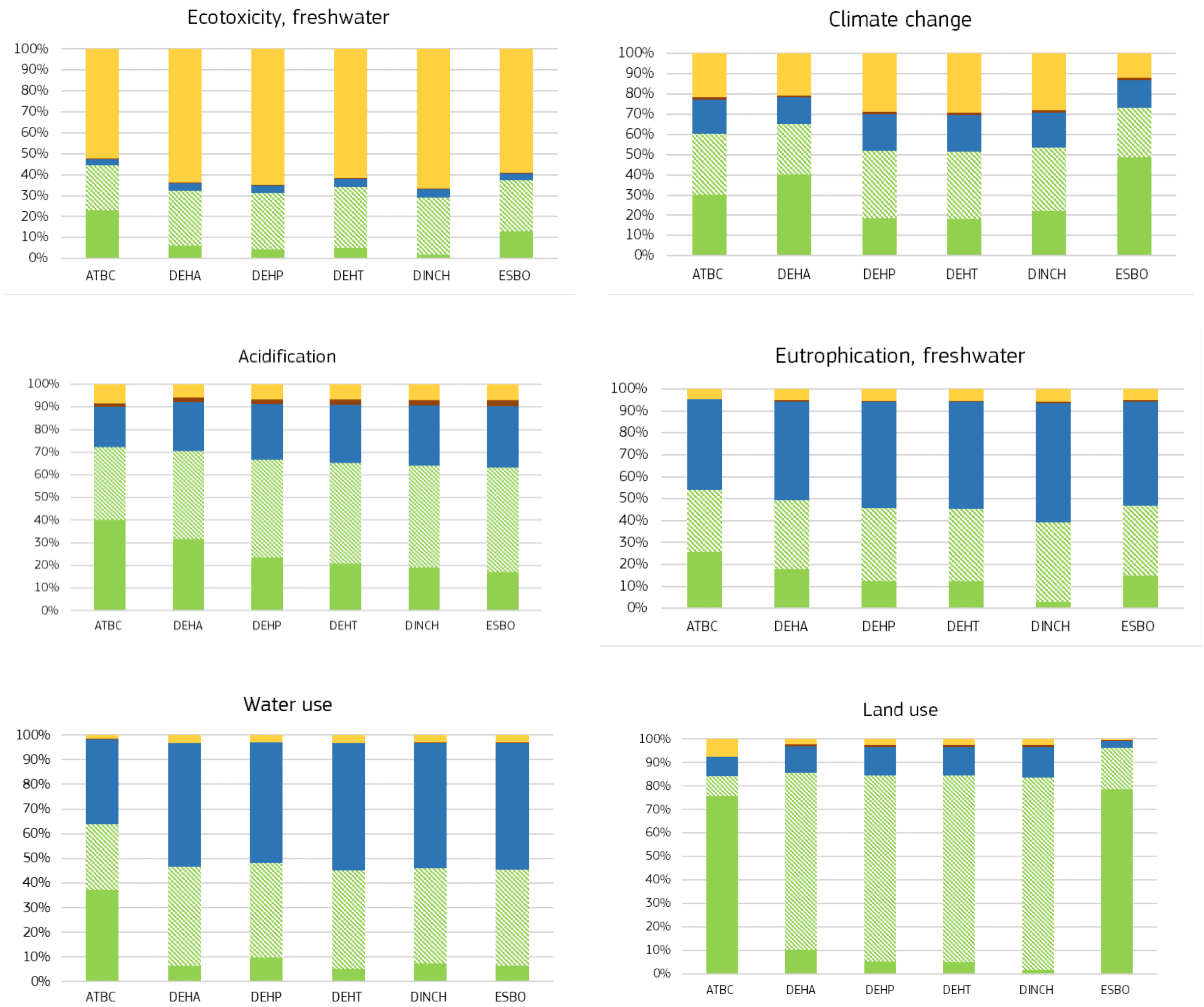
Figure A 8 shows the life cycle stages in the relevant impact categories identified in Table A 46, and the associated contribution. Percentages are presented in Table A 49.

Following the method reported in EC (2021), the most relevant stages include those that together contribute to at least 80% of the total characterised life cycle impact in the specific category.

For a more exhaustive picture, the contribution of all life cycle stages is listed as follows:

- Raw material acquisition stage contributes for all the relevant impact categories and for all six gaskets.
- Manufacturing stage contributes for all the gasket for the following impact categories: Resources use, fossil; Eutrophication, fresh water; Water use; Acidification. There is an exception for DINCH, as in this case the contribute of the manufacturing stage is limited, because more than 80% is already accounted in the Raw Material acquisition.
- Distribution stage does not account for any of the impact categories in any of the eight impact categories identified.
- End-of-life stage accounts for all six gaskets for Climate Change and Ecotoxicity, freshwater. The only exception is for DEHA gasket, in which EoL contributes on in the Ecotoxicity impact category.

Figure A 8. Contribution of each life cycle stage in relevant impact categories. The contribution of raw material acquisition is split in the contribution related to the plasticiser (green) and on related to PVC and additives (green diagonal pattern).



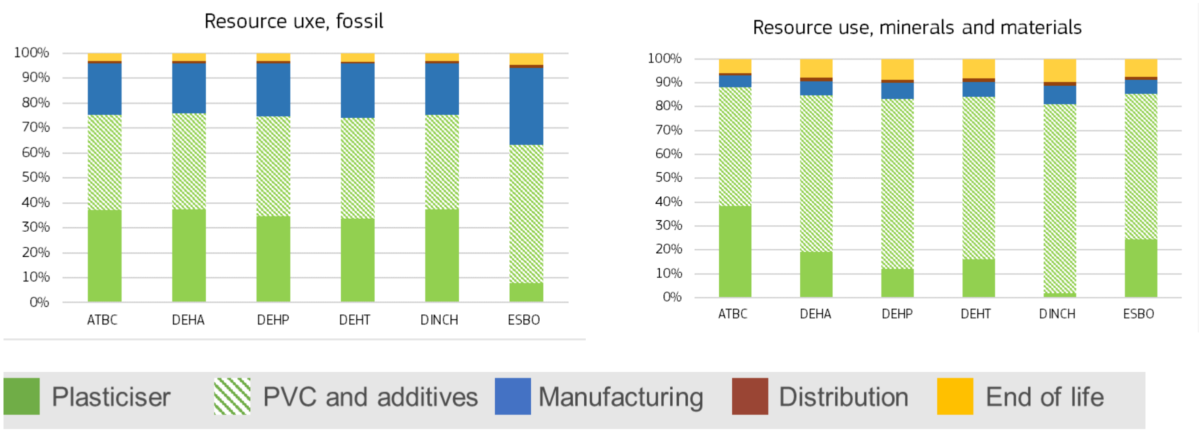

Resource uxe, fossil
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
ATBC
DEHA
DEHP
DEHT
DINCH
ESBO
Resource use, minerals and materials
100%
90%
80%
70%
60%
50%
40%
30%
20%
10%
0%
ATBC
DEHA
DEHP
DEHT
DINCH
ESBO
Plasticiser
PVC and additives
Manufacturing
Distribution
End of life

Table A 49. Most relevant life cycle stage identification for each impact category

DEHP	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	52.06%	74.58%	83.31%	31.19%	45.87%	48.12%	84.60%	66.59%
Plasticiser	18.58%	34.67%	12.05%	4.48%	12.56%	9.76%	5.37%	23.49%
PVC+Additives	33.48%	39.91%	71.26%	26.71%	33.31%	38.36%	79.23%	43.10%
Manufacturing	18.08%	21.30%	6.60%	3.55%	48.24%	48.84%	12.05%	24.56%
Distribution	1.21%	0.88%	1.44%	0.41%	0.56%	0.07%	0.87%	2.26%
End-of-life	28.65%	3.24%	8.65%	64.85%	5.33%	2.97%	2.48%	6.59%
ATBC	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	60.47%	75.23%	88.19%	44.59%	53.67%	63.53%	90.16%	75.20%
Plasticiser	30.09%	37.14%	38.40%	23.16%	25.76%	37.15%	87.87%	41.10%
PVC+Additives	30.38%	38.10%	49.79%	21.44%	27.91%	26.38%	10.12%	32.92%
Manufacturing	16.79%	20.80%	4.72%	2.91%	41.36%	34.37%	9.41%	18.03%
Distribution	1.12%	0.86%	1.03%	0.34%	0.02%	0.05%	0.11%	1.76%
End-of-life	21.61%	3.10%	6.06%	52.16%	4.49%	1.54%	8.63%	8.54%
DEHA	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	65.27%	75.93%	84.80%	32.38%	49.51%	46.63%	85.67%	70.52%
Plasticiser	40.14%	37.33%	19.17%	6.11%	17.75%	6.26%	10.39%	31.74%
PVC+Additives	25.13%	38.60%	65.64%	26.27%	31.76%	40.37%	75.28%	38.79%
Manufacturing	13.25%	20.11%	5.94%	3.40%	44.89%	50.16%	11.17%	21.58%
Distribution	0.89%	0.83%	1.29%	0.40%	0.52%	0.08%	0.80%	1.98%
End-of-life	20.60%	3.13%	7.97%	63.82%	5.08%	3.12%	2.36%	5.92%
DINCH	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	53.54%	75.22%	81.13%	29.21%	39.28%	46%	83.65%	64.11%
Plasticiser	22.32%	37.46%	1.97%	1.83%	3.04%	7%	1.93%	19.13%
PVC+Additives	31.21%	37.76%	79.16%	27.38%	36.24%	39%	81.72%	44.98%
Manufacturing	17.44%	20.84%	7.59%	3.76%	54.28%	51%	12.85%	26.51%

Distribution	1.17%	0.86%	1.65%	0.44%	0.63%	0%	0.92%	2.44%
End-of-life	27.86%	3.08%	9.63%	66.60%	5.81%	3%	2.57%	6.94%
DEHT	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	73.28%	63.37%	85.41%	37.32%	46.75%	45.41%	96.41%	63.13%
Plasticiser	48.78%	7.72%	24.27%	13.06%	15.06%	6.43%	78.53%	17.00%
PVC+Additives	24.50%	55.65%	61.14%	24.25%	31.69%	38.98%	17.88%	46.12%
Manufacturing	13.73%	30.82%	5.88%	3.34%	47.62%	51.50%	2.82%	27.28%
Distribution	0.92%	1.28%	1.28%	0.39%	0.55%	0.08%	0.20%	2.51%
End-of-life	12.07%	4.54%	7.43%	58.95%	5.08%	3.02%	0.56%	7.09%
ESBO	**Climate change, total**	**Resource use, fossil**	**Resource use, minerals and metals**	**Ecotoxicity, freshwater**	**Eutrophication, freshwater**	**Water use**	**Land use**	**Acidification**
Raw Material Acquisition	51.44%	74.09%	83.98%	31.32%	45.51%	45.22%	84.42%	65.28%
Plasticiser	17.99%	33.86%	15.99%	4.68%	12.35%	5.19%	5.14%	20.95%
PVC+Additives	33.45%	40.23%	67.99%	26.64%	33.16%	40.03%	79.28%	44.32%
Manufacturing	18.30%	21.74%	6.38%	3.58%	48.62%	51.60%	12.21%	25.58%
Distribution	1.22%	0.90%	1.39%	0.42%	0.56%	0.08%	0.88%	2.35%
End-of-life	27.86%	3.08%	9.63%	66.60%	5.81%	1.00%	2.57%	6.94%

A8.4.3 Identification of most relevant processes

The procedure for the selection of the most relevant processes is described in the PEF method (EC, 2021a). The most relevant processes are identified selecting the ones that together contribute to at least 80% of the total characterised life cycle impact in the specific category.

The PVC production, electricity and the precursor's production are the most relevant processes for the *Resource use, fossil impact category*. The relevant processes are: PVC production, Electricity and the plasticisers precursors for *Eutrophication, freshwater*. The most relevant processes are mainly the incineration of PVC, along with the production of Stearic acid for all six gaskets *Ecotoxicity, freshwater*. In *water use impact category,* the compounding process is as the first contributor to all six gaskets. Regarding *Resource use, minerals and materials*, the most relevant processes are mainly the production of PVC, along with incineration of PVC and the precursor production for all six gaskets, for the exception of DINCH. For this latter, the precursors do not contribute to the 80% of the impact. Similarly, PVC production is the main process contributing to *Acidification*. For *Land Use*, the contributions are different depending on the kind of gaskets. In the case of those made from natural resources: for ATBC only the precursor Citric acid accounts for more than 89%; whilst for ESBO along with the precursor of the plasticiser Soybean oil, there is a contribute from Stearic acid. On the other hand, for the case of petrol-based gaskets, Stearic acid is one the most relevant process that standalone for more than 60%. The other most relevant processes for DEHA, DEHP, DEHT and DINCH are Electricity and PVC production, with the exception of DINCH, in which instead PVC production does not account.

Table A 50 shows the processes which contribute (along the entire life cycle) more than 80% to the Climate Change impact category highlighting the values in bold with coloured background. The different coloured backgrounds are used to identify in which life cycle stage they appear. Dark green background is referred to the manufacturing of the plasticisers; light green background indicates the processes related to PVC and additives manufacturing; blue background represents the processes of the manufacturing of the gaskets; and yellow background refers to EoL processes.

Table A 50 shows that the production of the PVC and electricity contributes to all six gaskets. For each gasket, also the precursors for the production of the plasticisers are identified as the most relevant processes, except for Hydrogen and Hydrogen peroxide productions, respectively for DINCH and ESBO. Finally, also some processes from End-of-life are spotted. In particular, the incineration of PVC and the incineration of the plasticiser itself also account, with the exception for DEHT and ESBO gaskets, while in the case of ATBC gasket is relevant only the incineration of PVC.

Table A 50. Most relevant processes for impact category Climate change, total. Colours refer to the life cycle stage as depicted in Figure 1

Process	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**24.6%**	**20.4%**	**27.2%**	**36.9%**	**25.3%**	**19.9%**
Electricity, medium voltage {RER}|	**16.6%**	**13.4%**	**18.3%**	**22.1%**	**17.6%**	**13.6%**
Waste polyvinylchloride {CH}| treatment of municipal incineration	**12.7%**	**10.5%**	**14.0%**	3.1%	**13.1%**	10.3%
Waste plasticiser municipal incineration	6.7%	**8.2%**	**12.2%**		**12.5%**	
Soybean oil, crude {RER}| soybean meal and crude oil production						**46.7%**
Propylene {RER}| market for propylene		4.1%	**5.5%**	**12.6%**		
Phthalic anhydride {RER}| production			**7.5%**			
DINP_Ecoprofile					**18.8%**	
Purified terephthalic acid {RER}| production				**10.4%**		
Adipic acid {RER}| production		**32.0%**				
Citric acid {RER}| production	**11.3%**					

1-butanol {RER}| hydroformylation of propylene	**10.6%**					
Acetic anhydride {RER}| production, ketene route	**7.3%**					
Carbon monoxide {RER}| production			3.0%	6.7%		
Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated	3.1%	2.6%	3.4%	1.8%	3.2%	2.5%
Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation				2.4%		
Hydrogen peroxide, without water, in 50% solution state {RER}| hydrogen peroxide production, product in 50% solution state						1.6%

Table A 51 shows the processes contributions for the Resource use, fossil impact category. Similarly to the Climate Change, the PVC production, electricity and the precursor's production are the most relevant processes. However, in this category along with Hydrogen and Hydrogen peroxide production also Carbon monoxide, Acetic Anhydride and Soybean oil production do not account. On the other hand, the End-of-life processes are not present.

Similarly, in Table A 52 Eutrophication, freshwater, the relevant processes are PVC production, Electricity and the plasticisers precursors. For these latter the relevant ones are: carbon monoxide, soybean oil, adipic acid, citric acid and butanol respectively for their corresponding plasticisers.

Table A 51. Most relevant processes for impact category Resource use, fossil

Process	**ATBC**	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**35.0%**	**35.4%**	**36.7%**	**36.9%**	**34.7%**	**51.1%**
Electricity, medium voltage {RER}|	**20.6%**	**20.5%**	**21.7%**	**22.1%**	**21.2%**	**30.7%**
Propylene {RER}| market for propylene		**11.6%**	**12.2%**	**12.6%**		
DINP_Ecoprofile					**33.8%**	
Phthalic anhydride {RER}| production			**12.0%**			
Carbon monoxide {RER}		6.1%	6.4%	6.7%		
Purified terephthalic acid {RER}| production				**10.4%**		
Adipic acid {RER}| production		**15.8%**				
1-butanol {RER}| hydroformylation of propylene	**18.6%**					
Citric acid {RER}| production	**9.2%**					
Waste polyvinylchloride {CH}| treatment of municipal incineration	2.91%	2.94%	2.4%	3.07%	2.9%	
Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated	1.67%	1.7%	1.75%	1.8%	1.7%	4.2%
Hydrogen, gaseous {Europe without Switzerland}| hydrogen production, gaseous, petroleum refinery operation		2.2%	2.4%	2.4%		
Acetic anhydride {RER}| production, ketene route	8.7%					
Soybean oil, crude {RER}| soybean meal and crude oil production						3.8%

Table A 52. Most relevant processes for impact category Eutrophication, freshwater

Process	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Electricity, medium voltage {RER}| market group for	**41.4%**	**46.1%**	**49.5%**	**50.0%**	**55.6%**	**47.9%**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**23.5%**	**26.7%**	**28.0%**	**27.9%**	**30.5%**	**26.6%**
Carbon monoxide {RER}		5.0%	**7.0%**	**7.2%**		
Soybean oil, crude {RER}| soybean meal and crude oil production						**12.3%**
Adipic acid {RER}| production		**9.3%**				
Citric acid {RER}| production	**11.8%**					
1-butanol {RER}| hydroformylation of propylene	**8.2%**					
Acetic anhydride {RER}| production, ketene route	5.5%					
Waste polyvinylchloride {CH}| treatment of, municipal incineration			5.2%		5.7%	

In the case of the category Ecotoxicity, freshwater, Table A 53, the most relevant processes are mainly the incineration of PVC, along with the production of Stearic acid for all six gaskets. PVC production is also identified Most relevant process for DEHA, DEHP and DEHT gaskets. Finally, the precursors are also relevant for only ATBC and ESBO with respectively Citric Acid and Acetic Anhydride for the first gasket, and Soybean oil for the latter gasket.

Table A 53. Most relevant processes for impact category Ecotoxicity, freshwater

Process	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Waste polyvinylchloride {CH}| treatment of municipal incineration	**50.9%**	**62.3%**	**63.4%**	**63.2%**	**65.1%**	**57.6%**
Stearic acid {GLO}| stearic acid production	**12.4%**	**15.2%**	**15.4%**	**15.4%**	**15.8%**	**14.0%**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	7.1%	**8.7%**	**8.8%**	**8.8%**	9.1%	8.0%
Citric acid {RER}| production	**11.3%**					
Acetic anhydride {RER}| production, ketene route	**9.3%**					
Soybean oil, crude {RER}| soybean meal and crude oil production						**12.4%**
Electricity, medium voltage {RER}	2.9%	3.5%	3.6%	3.7%	3.8%	3.3%
Adipic acid {RER}| production		2.6%				

Table A 54. Most relevant processes for impact category Water use

Processes	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Compounding	**31.4%**	**45.9%**	**46.9%**	**47.2%**	**46.0%**	**47.1%**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**24.8%**	**38.0%**	**37.9%**	**37.7%**	36.0.2%	**36.7%**
DINP_Ecoprofile					**7.2%**	
Citric acid {RER}| production	**14.4%**					
1-butanol {RER}| hydroformylation of propylene	**12.1%**					
Electricity, medium voltage {RER}		4.4%	4.5%	4.6%	4.4%	

In water use impact category (Table A 54), the compounding process is as the first contributor to all six gaskets. This is linked to the large amount of cooling water used during step.

PVC production is always among the most relevant processes with exception to DINCH gaskets. For DINCH is paramount the water used in the DINP production, which is the precursor of the plasticiser. Also, in ATBC gasket, two of the precursors contribute to this impact category.

Table A 55 shows the results for Resource use, minerals and materials. The most relevant processes are mainly the production of PVC, along with incineration of PVC and the precursor production for all six gaskets, for the exception of DINCH. For this latter, the precursors do not contribute to the 80% of the impact. Also the production of stearic acid and electricity contribute to the impact for almost all the gaskets, with the exceptions of ESBO for electricity and ATBC for none of these latter two processes.

Table A 55. Most relevant processes for impact category Resource use, minerals and materials

Process	**ATBC**	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**39.1%**	**51.6%**	**56.0%**	**53.4%**	**62.2%**	**48.0%**
Waste polyvinylchloride {CH}| treatment of, municipal incineration	**5.9%**	**7.8%**	**8.5%**	**8.1%**	**9.4%**	**7.3%**
Stearic acid {GLO}| stearic acid production	5.1%	**6.7%**	**7.3%**	**7.0%**	**8.1%**	**6.3%**
Electricity, medium voltage {RER}	4.7%	**6.1%**	**6.8%**	**6.6%**	**7.8%**	5.9%
Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated		5.5%	5.9%	5.7%	6.6%	5.1%
Phthalic anhydride {RER}| production			**5.9%**			
Purified terephthalic acid {RER}| production				**10.0%**		
Adipic acid {RER}| production		**13.7%**				
Citric acid {RER}| production	**20.0%**					
1-butanol {RER}| hydroformylation of propylene	**9.4%**					
Acetic anhydride {RER}| production, ketene route	**8.7%**					
Soybean oil, crude {RER}| soybean meal and crude oil production						**20.6%**

Table A 56. Most relevant processes for impact category Acidification

Process	**ATBC**	**DEHA**	**DEHP**	**DEHT**	**DINCH**	**ESBO**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	**24.4%**	**28.7%**	**31.9%**	**53.4%**	**33.3%**	**34.2%**
Electricity, medium voltage {RER}	**19.1%**	**22.0%**	**25.0%**	**6.6%**	**27.0%**	**27.3%**
Stearic acid {GLO}| stearic acid production	5.3%	**6.2%**	**6.9%**	**7.0%**	**7.2%**	**7.4%**
Waste polyvinylchloride {CH}| treatment of, municipal incineration	4.6%	**5.4%**	**6.0%**	**8.1%**	6.26%	6.4%
Phthalic anhydride {RER}| production			**9.6%**			
Carbon monoxide {RER}		**4.8%**	**5.5%**			
DINP_Ecoprofile					**13.6%**	
Adipic acid {RER}| production		**19.5%**				
Citric acid {RER}| production	**22.6%**					
1-butanol {RER}| hydroformylation of propylene	**10.7%**					
Acetic anhydride {RER}| production, ketene route	**7.1%**					
Soybean oil, crude {RER}| soybean meal and crude oil production						**14.0%**
Purified terephthalic acid {RER}| production				**10.0%**		
Propylene {RER}| production		3.8%	4.3%			
Calcium carbonate, precipitated {RER}| calcium carbonate production, precipitated	1.7%	2.0%	1.7%	5.67%	2.28%	2.34%

For Land Use (Table A 57) the contributions are different depending on the kind of gaskets. In the case of those made from natural resources: for ATBC only the precursor Citric acid accounts for more than 89%; whilst for ESBO along with the precursor of the plasticiser Soybean oil, there is a contribute from Stearic acid.

On the other hand, for the case of petrol-based gaskets, Stearic acid is one the most relevant process that standalone for more than 60%. The other most relevant processes for DEHA, DEHP, DEHT and DINCH are Electricity and PVC production, with the exception of DINCH, in which instead PVC production does not account.

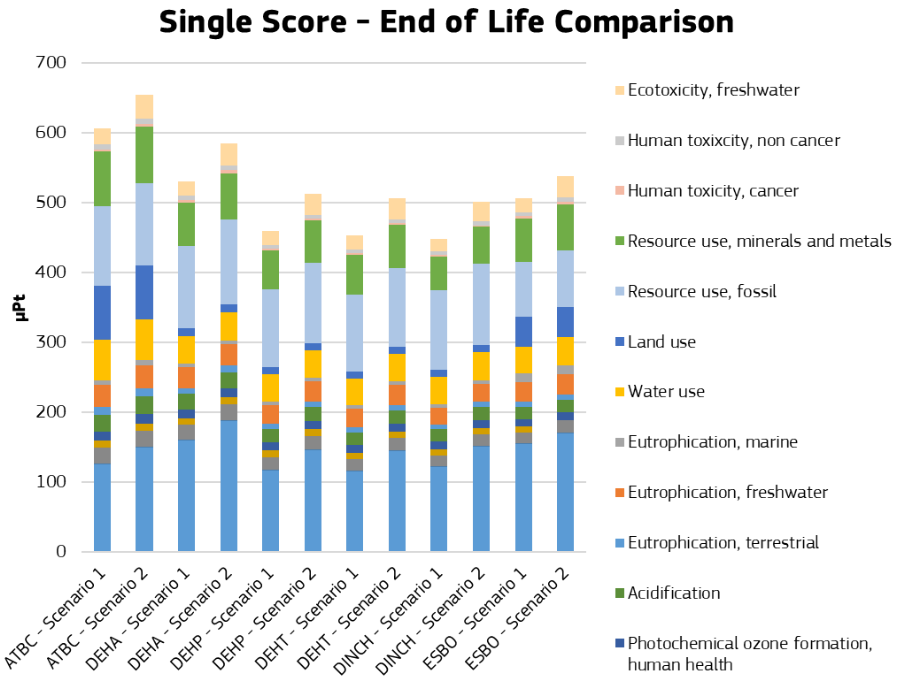
Table A 57. Most relevant processes for impact category Land use

Process	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Stearic acid {GLO}| stearic acid production	8.4%	**62.1%**	**65.4%**	**65.4%**	**67.4%**	**14.8%**
Electricity, medium voltage {RER}	1.6%	**11.5%**	**12.4%**	**12.5%**	**13.2%**	**2.8%**
Polyvinylchloride, emulsion polymerised {RER}| polyvinylchloride production, emulsion polymerisation	1.5%	**11.1%**	**11.7%**	**11.7%**	12.0%	**2.6%**
Citric acid {RER}| production	**86.8%**					
1-butanol {RER}| hydroformylation of propylene	0.6%					
Acetic anhydride {RER}| production, ketene route	0.5%					
Soybean oil, crude {RER}| soybean meal and crude oil production						**78.3%**
Carbon monoxide {RER}| production			2.4%	2.5%		
Waste polyvinylchloride {CH}| treatment of, municipal incineration		2.3%	2.2%	2.2%	2.25%	6.4%
Adipic acid {RER}| production		7.1%				

A.8.4.4 Comparing End-of-life Scenarios

Figure A 9 presents the results (single score) for the EoL scenarios considered, Scenario 1 with a share of 53% incineration and 43% landfill, and Scenario 2 with 100% to incineration. For all the six gaskets the impact of scenario 2 is higher than scenario 1. The main differences can be spotted for “climate change” and “ecotoxicity, freshwater” impact categories due to highest emission to air of the incineration processes compared to the landfill ones. This is also observed for each individual impact category at a slighter extent.

Figure A 9. Cradle to grave single score results for the six gaskets: Comparison of two End-of-life scenario



A8.4.5 Data quality and uncertainty assessment

The data quality assessment of the data used was done following the procedure defined in the PEF method to assess the compliance of the EF datasets, in which four data quality criteria are defined in EC (2021): Technological Representativeness (TeR), Geographical Representativeness (GeR), Time-related Representativeness (TiR), and Precision (P). Each data quality criterion is rated according to five levels, from *excellent* to *poor,* and to five corresponding scores, from *1* to *5* as presented in Table A 58. The four criteria scores are averaged, and the data quality score (DQR) is obtained. The overall DQR ranges are presented in Table A 59.

DQR is applicable to company-specific datasets and secondary datasets. In case of secondary dataset the quality is attributed by rating both the dataset and the related activity data. Company specific datasets rates are the weighted average of the rating of the most relevant processes or elementary flows that are part of the dataset.

Table A 58. Data quality score levels, adapted from EC (2021)

Overall DQR	Overall data quality level
DQR ≤ 1.5	'Excellent quality'
1.5 < DQR ≤ 2.0	'Very good quality'
2.0 < DQR ≤ 3.0	'Good quality'
3 < DQR ≤ 4.0	'Fair quality'
DQR >4	'Poor quality'

Table A 59 presents the result of the data quality rating. It is important to highlight the PEF method refers only to the evaluation of the normalized and weighted results, which are reported in the first row. A *good quality* of the dataset is obtained for all the six gaskets.

In this analysis are also assessed the DQR of the most relevant impact categories previously identified. Also, for the single impact categories the results are at level of *good quality* for all the gaskets, with better performance, *very good quality*, for water use, Resource use, minerals and materials for all the gasket, while for acidification only for ATBC and DINCH, instead in the case of Land use DEHA, DEHT, DINCH and ESBO have also *very good quality.*

Table A 59. Results of the data quality rating (DQR) for single score and the most relevant impact categories of Hot Spot Analysis, following the data quality score levels in Table A 58.

	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Single Score	2.14	2.03	2.07	2.07	2.34	2.07
Climate change, total	2.21	2.32	2.14	2.24	2.05	2.02
Resource use, fossil	2.13	2.19	2.00	2.10	2.02	2.03
Eutrophication, freshwater	2.17	2.19	2.17	2.21	2.23	2.20
Ecotoxicity, freshwater	2.34	2.38	2.38	2.29	2.45	2.39
Water use	1.88	1.82	1.87	1.82	1.98	1.57
Resource use, minerals and materials	1.93	1.90	1.82	1.84	1.91	1.62
Acidification	1.75	2.04	2.29	2.29	2.00	2.02
Land use	2.00	1.85	2.02	1.85	1.87	1.96

Annex 9. Step 4 – Normalization (EF and Planetary boundaries) and weighting factors (EF)

Table A 60. Sets of normalisation and weighting factors used across the study

Impact category	EF normalization factors	EF weighting factors (%)	PB normalization factors
Human toxicity, cancer	1.19E+05	2.13	9.62E+05
Human toxicity, non-cancer	8.88E+05	1.84	4.10E+06
Ecotoxicity, freshwater	3.91E+14	1.92	1.31E+14
Climate change	5.21E+13	21.06	6.81E+12
Ozone depletion	3.61E+08	6.31	5.39E+08
Particulate matter	4.11E+06	8.96	5.16E+05
Ionizing radiation, Human health	2.91E+13	5.01	5.27E+14
Photochemical ozone formation, human health	2.82E+11	4.78	4.07E+11
Acidification	3.83E+11	6.20	1.00E+12
Eutrophication, terrestrial	1.22E+12	3.71	6.13E+12
Eutrophication, freshwater	1.11E+10	2.80	5.81E+09
Eutrophication, marine	1.35E+11	2.96	2.01E+11
Land use	5.65E+15	7.94	5.21E+15
Water use	7.91E+13	8.51	1.82E+14
Resource use, minerals and metals	4.39E+08	7.55	2.19E+08
Resource use, fossil	4.48E+14	8.32	2.24E+14

Additional method for absolute sustainability assessment

In this case study, we tested two methods, one provides carrying capacity-based normalisation references for the EF midpoint categories (Sala et al., 2020) and it is reported in chapter 2.2.4.4. Another approach, is based on PB-informed characterisation models defining characterisation factors (CFs) to map the elementary flows onto the control variables (Ryberg et al., 2018, 2021) both using currently generic carrying capacities where spatialized factors are not yet available (e.g. for chemical pollution and related toxicity and ecotoxicity). For the latter, a planetary boundary transgression level (Tulus et al., 2021) was defined based on the sharing principles 'equal per capita' (downscale to individual level) and gross value added (GVA; upscale to product level). However, a key challenge in the application of this method is to determine the allocation of the Safe Operating Space to the chemical/material under assessment. The result of this approach is reported hereunder.

PB-informed characterisation models and allocation of the Safe Operational Space

To perform a sensitivity assessment, another method has been applied to estimate the impact of plasticizers on planetary boundaries. As described in Box 2, this requires allocating a share of the global ecological budget, referred to as safe operating space (SOS), to a given product. The impact of the chemical is then evaluated against such reference limit, shedding light on whether it operates sustainably within the allowable budget or unsustainably (if it transgresses it). In what follows, a detailed description of the calculations is provided and some results, while further details can be found in the original publications. We note that we report preliminary results, which will be refined further.

Box 2. Description of the method for AESA based on Tulus et al. (2021)

Method

In this approach the life cycle impact assessment, was performed using the absolute environmental sustainability impact assessment (AESA) method developed by Ryberg et al. (2018) and complemented by Galán-Martín et al. (2021). The current version of the AESA method is implemented as a python package for use within the Brightway2 framework.

Next, the results obtained with the AESA method were put into perspective by comparison with their downscaled safe operating space (SOS), leading to a specific value of a transgression level (TL).

In mathematical terms, the TL of scenario *s* in the category of a PB *b* is computed as shown in (1), where IMP_{bs} denotes the total impact of scenario *s* in the PB *b* and $shareSOS_{bs}$ denotes the downscaled SOS assigned to scenario *s*. *B* is the set of nine control variables (categories) for the PBs, and *S* is the set of six gasket production scenarios (ATBC, DEHA, DEHP, DEHT, DINCH and ESBO), described elsewhere.

$$TL_{bs} = \frac{IMP_{bs}}{shareSOS_{bs}} \quad \forall b \in B, s \in S \tag{1}$$

For a TL below one, a scenario could be deemed environmentally sustainable, whereas any TL above one would indicate that the scenario operates unsustainably considering its allocated share of the PB.

The procedure for SOS downscaling, presented next, is based on the methods described in Tulus et al. (2021). The downscaling of SOS follows the equality principle (i.e., Equal Per Capita, EPC), assuming that every person has the same moral right to access the Earth's ecological budget. This personal share of the SOS is then upscaled to each alternative gasket production scenario based on the economic value of the latter (considering the economic value as a valid proxy for human wellbeing). Hence, the general equation for the share of the SOS of a scenario *s* is as follows:

$$shareSOS_{bs}^{EPC} = \frac{SOS_b}{pop^{TOT}} pop_s \frac{price_s \cdot DEM_s}{GVA^{TOT \rightarrow pop_s}} \quad \forall b \in B, s \in S \tag{2}$$

Where SOS_b is the total SOS within PB *b*, pop^{TOT} is the total world population, pop_s is the population that benefits from the use of the gaskets *s*, $price_s$ is the unitary market price of gasket *s*, DEM_s is the total demand of gaskets *s* from pop_s and $GVA^{TOT \rightarrow pops}$ is the GVA of all economic activities that benefit pop_s. Combining and reorganizing (1) and (2), we get (3).

$$TL_{bs}^{EPC} = \frac{IMP_{bs}}{shareSOS_{bs}} = \frac{imp_{bs} \cdot DEM_s}{\dfrac{SOS_b \cdot pop_s \cdot price_s \cdot DEM_s}{pop^{TOT} \cdot GVA^{TOT \rightarrow pop_s}}} = \frac{imp_{bs} \cdot pop^{TOT} \cdot GVA^{TOT \rightarrow pop_s}}{SOS_b \cdot pop_s \cdot price_s} \quad \forall b \in B, s \in S \tag{3}$$

Results

The assumption that DEM_s corresponds to the amount of produced (and consumed) gaskets in one specific year within the EU-27 region allows simplifying the calculations as shown in (3). We were unable to obtain accurate prices data, so we carried out the calculations assuming a unitary price of 1 €/kg for each gasket produced in scenario *s* and gathering the GVA and population data for 2021.[12] Following this approach, the TL of the alternative scenarios can be obtained, as displayed in Table A 61. As seen, most of the PBs are heavily transgressed according to the above assumptions. This was expected as chemicals are mostly based on fossil carbon, and they also consume fossil resources during chemical transformations, leading to large CO_2 emissions that strongly impact on the PBs, particularly those more strongly connected to carbon emissions (e.g., climate change, ocean acidification and biosphere integrity).

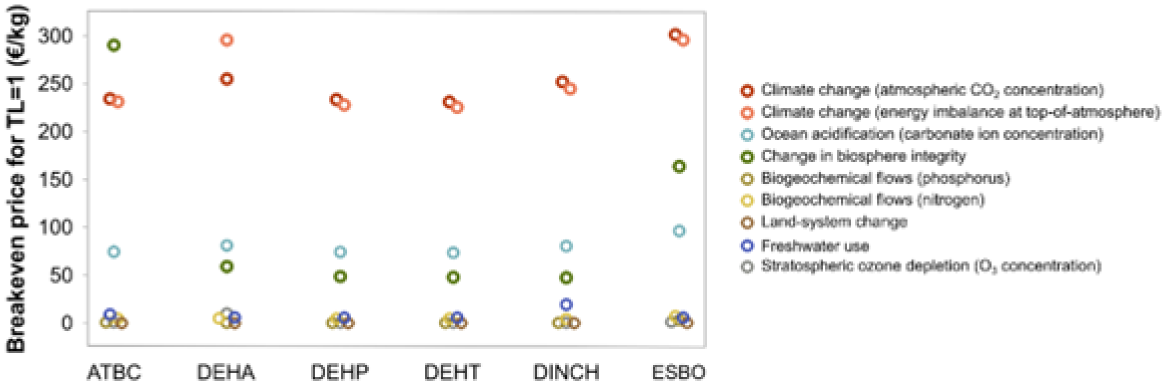
Table A 61. Transgression levels for the set of alternative gasket production scenarios for each control variable of the PB framework.

	ATBC	DEHA	DEHP	DEHT	DINCH	ESBO
Climate change (atmospheric CO_2 concentration) (ppm)	234	255	233	231	252	301
Climate change (energy imbalance at top-of-atmosphere) (W/m^2)	231	296	228	225	245	296
Stratospheric ozone depletion (O_3 concentration) (Dobson unit)	0.9	10.4	0.4	0.4	0.4	1.4
Ocean acidification (carbonate ion concentration) (Ω aragonite)	75	81	74	74	80	96
Biogeochemical flows (phosphorus) (Tg P)	0.9	0.3	0.3	0.3	0.2	3.2
Biogeochemical flows (nitrogen fixation) (Tg N)	5	5	5	5	5	7
Land-system change (% forested land)	0.01	0.01	0.01	0.01	0	0.23
Freshwater use (km^3)	9	6	6	6	20	6
Change in biosphere integrity (% BII loss)	291	59	49	48	48	164

Values above one (in red) indicate environmentally unsuitable scenario, values equal or below one (in green) indicate that the scenario is environmentally sustainable (i.e., the production of the gasket is performed within the allocated share of safe operating space).

Because the prices used in the calculations were not fully precise, we computed the ranges of breakeven prices that would make the gasket production scenarios environmentally sustainable (TL=1), as shown in Figure 15 Prices above 300 €/kg of gasket could provide absolute environmental sustainability for every category of the PB framework. However, these results are subject to the set of aforementioned assumptions, which –as already mentioned– will be refined in the future.

Figure A 10. Range of breakeven prices for the set of alternative gasket production scenarios for each control variable of the PB framework.



Annex 10. Background data for the socio-economic sustainability assessment

Table A 62. List of indicators to assess the foreground system. Source: (UNEP, 2021)

Stakeholder category	Social impact sub-categories	Examples of indicators for foreground process (KPI for companies)	Unit
Workers	Child labour	Percentage of working children under the legal age or 15 years old	%
Workers	Fair salary	Lowest paid worker, compared to the minimum wage and/or living wage	EUR
Workers	Forced labour	Workers voluntarily agree upon employment terms. Employment contracts stipulate wage, working time, holidays, and terms of resignation. Employment contracts are comprehensible to the workers and are kept on file	text
Workers	Health and Safety	Number of injuries or fatal accidents in the organization by job qualification inside the company	Number of accident in a certain timeframe
Workers	Health and Safety	Presence of a formal policy concerning health and safety	Text and reference
Workers	Health and Safety	Preventive measures and emergency protocols exist regarding accidents and injuries	Text and reference
Workers	Health and Safety	Preventive measures and emergency protocols exist regarding chemical exposure	Text and reference
Workers	Health and Safety	Number of (serious/non-serious) Occupational Safety and Health Administration (OSHA) violations reported within the past 3 years and status of violations	Text
Workers	Health and Safety	Education, training, counselling, prevention, and risk control programs in place to assist workforce members, their families, or community members regarding serious disease	Text
Workers	Freedom of association and collective bargaining	Presence of unions within the organization is adequately supported (availability of facilities to union, posting of union notices, time to exercise the representation functions on paid work hours)	Text
Workers	Freedom of association and collective bargaining	Check the availability of collective bargaining agreement and meeting minutes (e.g. copies of collective bargaining negotiations and agreements are kept on file)	Text
Workers	Freedom of association and collective bargaining	Employee/union representatives are invited to contribute to planning of larger changes in the company, which will affect the working conditions	
Workers	Working hours	Number of hours effectively worked by employees (at each level of employment)	Hours/week
Workers	Working hours	Number of holidays effectively used by employees (at each level of employment)	Days/year
Workers	Working hours	Respect of contractual agreements concerning overtime	Yes/no
Workers	Working hours	The organization provides flexibility	Text
Workers	Equal opportunities / discrimination	Presence of formal policies on equal opportunities	Text and reference
Workers	Equal opportunities / discrimination	Ratio of basic salary of men to women by employee category	Ratio
Workers	Equal opportunities / discrimination	Composition of governance bodies and breakdown of employees per category according to gender, age group, minority, group membership, and other indicators of diversity	Text
Local community	Community engagement	Number and quality of meetings with community stakeholders	Text
Local community	Community engagement	Diversity of community stakeholder groups that engage with the organization	Text

Stakeholder category	Social impact sub-categories	Examples of indicators for foreground process (KPI for companies)	Unit
Local community	Local employment	Percentage of workforce hired locally	%
Local community	Local employment	Strength of policies on local hiring preferences	Text
Local community	Local employment	Percentage of spending on locally-based suppliers	%
Local community	Respect of indigenous rights	Strength of policies in place to protect the rights of indigenous community members	text

Table A 63. Reference scales used for the social assessment (Eisfeldt, 2017; Maister et al., 2020)

		Unit	Very high risk	High risk	Medium risk	Low risk	Very low risk
Child labour	Children in employment, male	%	>10	5-10	2.5-5	1-2.5	<= 1
	Children in employment, female						
	Children in employment, total						
Fair salary	Living wage, per month		See Maister et al. 2020 for explanations on the risk assessment. Risk levels were retrieved from PSILCA v.3 database.				
	Minimum wage, per month						
	Sector average wage, per month						
Forced labour	Trafficking in persons	Tier	3	2.1	2	-	1
	Frequency of forced labour	%	≥ 1.2	0.6 -1.2	0.4 -0.6	0.2 -0.4	< 0.2
Health and Safety (workers)	Rate of non-fatal accidents at workplace	# per 100,000 employees	≤ 3000	2250 -3000	1500 - 2250	750 - 1500	0 - 750
	Rate of fatal accidents at workplace	# per 100,000 employees	≤ 40	25 -40	15-25	7.5 -15	0 -7.5
	DALYs due to indoor and outdoor air and water pollution	DALYs per 1000 inhabitants	>50	30-<50	15-<30	5-<15	>0-<5
	Presence of sufficient safety measures	Cases of violation per 100,000 employees	> 0.0565	0.0215 - < 0.0565	0.0095- < 0.0215	0.0025 - < 0.0095	< 0.0025
	Workers affected by natural disasters	% of population	>=10	5-<10	3-<5	1-<3	0-<1
	Violations of mandatory health and safety standards	number of cases / force labour	>=5e-6	1.5e-6-<5e-6	8e-7 -<1.5e-6	2.5e-7-<8e-7	5.5e-8-<2.5e-7
Freedom of association and	Trade union density	% of employees organized in trade unions	0-20%	20-40%	40-60%	60-80%	>80%
	Right to strike	Point scale	0	1	-	2	3

		Unit	Very high risk	High risk	Medium risk	Low risk	Very low risk
collective bargaining	Right to association	Point scale	0	1	-	2	3
	Right of collective bargaining	Point scale	0	1	-	2	3
Working hours	Weekly hours of work per employee	Hours per week	<20 and >60	20 - <30 and 55 - <60	30 - <40 and 48 - <55	40 - <48	-
Equal opportunities / discrimination	Women in the sectoral labour force	Ratio	<0.2	0.2-<0.4	0.4-<0.6	0.6-<0.8 or >1.5	0.8-<1 or >1-1.5
	Gender wage gap	%	>=30% and <=-30	20% - <30% and -20% - >-30%	10% - <20% and -10% - >-20%	5% - <10% and -5% - >-10%	0% - <5% and 0% - >-5%
Respect of indigenous rights	Presence of indigenous populations	Yes/no			Yes		No
	Indigenous people rights protection index	Point scale	1	2	3	4	5

Annex 11. Presentations on the case studies developed by industry

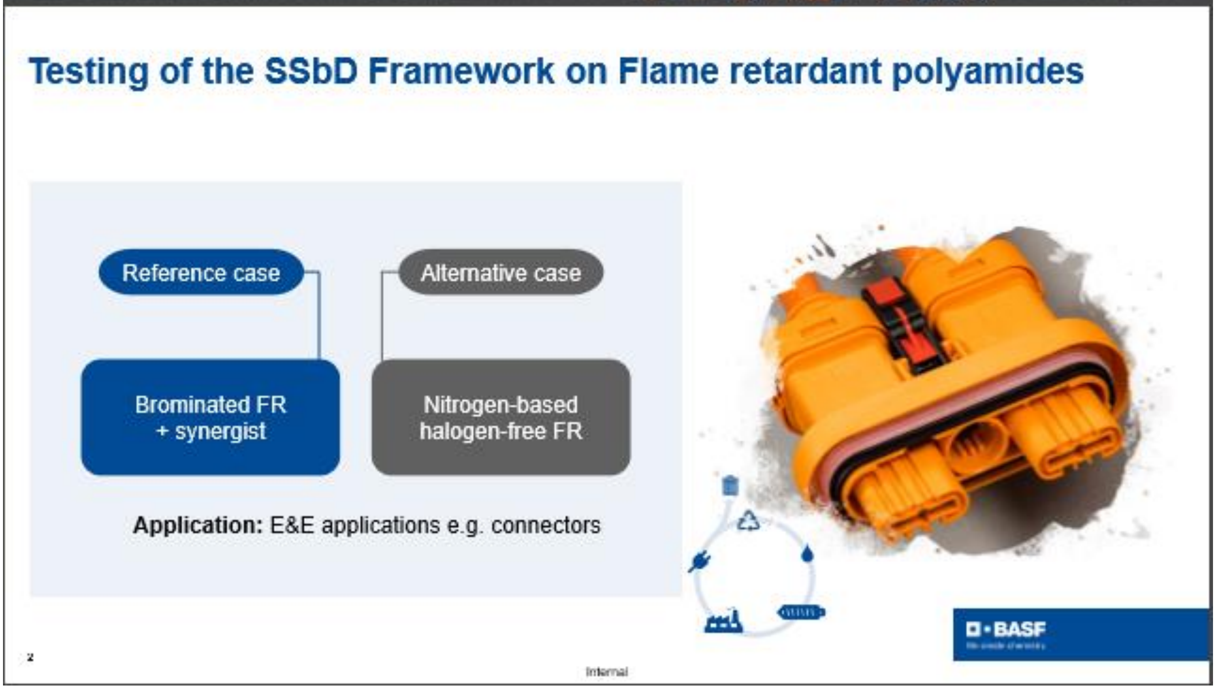
Case study 2: Flame retardants (halogen-free) in Information and communications technology (ICT) products

BASF Presentation

BASF
We create chemistry

Case Study
FR PA6: 'Safe & Sustainable by Design (SSbD)' Assessment

BASF – February 2023



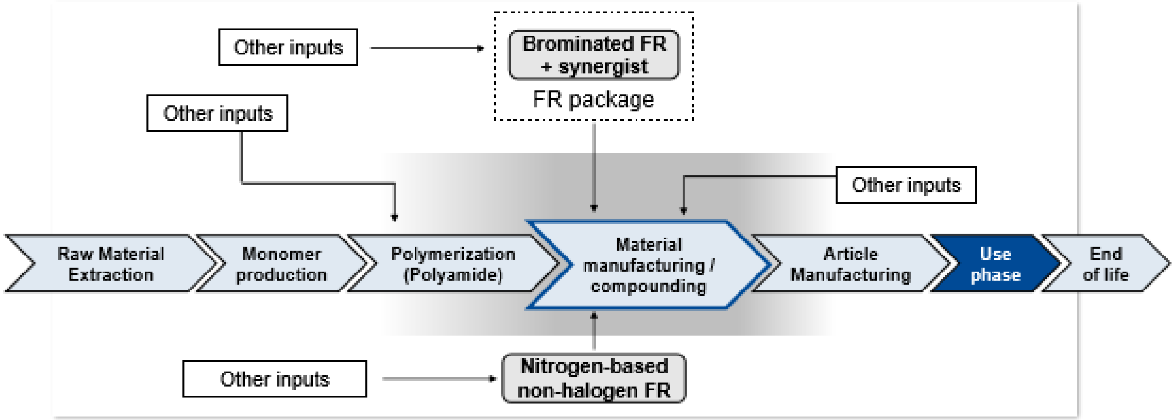
Testing of the SSbD Framework on Flame retardant polyamides

Reference case
Brominated FR + synergist

Alternative case
Nitrogen-based halogen-free FR

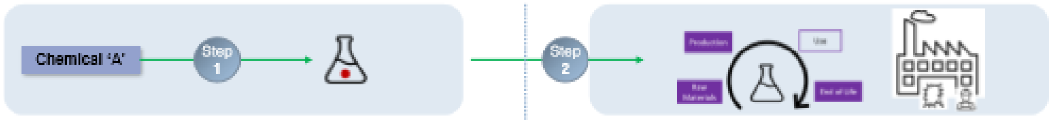
Application: E&E applications e.g. connectors

The production of FR based Polyamide is based on a multi-step value chain



SSbD assessment Steps

Approach, Challenges and Suggestions



Approach

Hazard assessment based on existing toxicological and eco-toxicological data e.g. from the respective REACH dossiers

- ➢ No additional animal tests at the value chain stage of a compound producing manufacturer proposed, which lead to data gaps

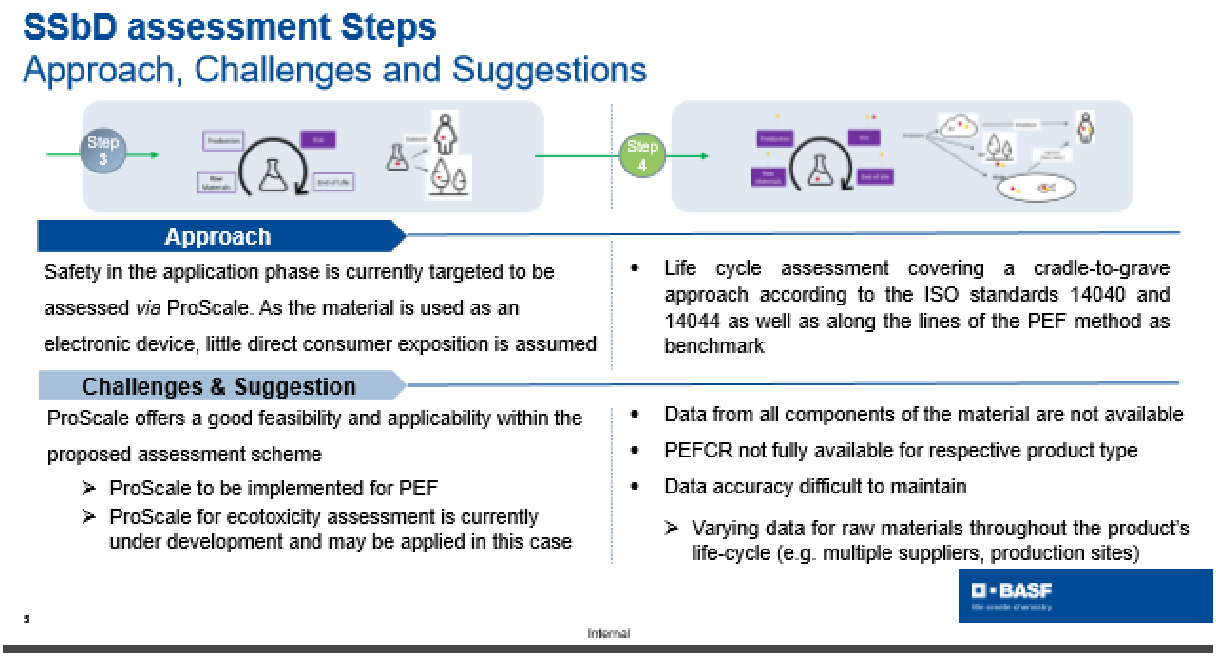
Assessment of safety aspects focusing on the chemical production along the value chain for instance based on ECETOC's Targeted Risk Assessment (TRA)

Challenges & Suggestion

Assessment depends on the step in the value chain

- ➢ Outcome of the assessment could vary, weather the evaluation is conducted on an early precursor, the applied flame retardant (chemical) itself or the resulting material

- Assessment step under evaluation
- Accurate data only available for own production step



SSbD assessment Steps

Approach, Challenges and Suggestions

Approach

Safety in the application phase is currently targeted to be assessed *via* ProScale. As the material is used as an electronic device, little direct consumer exposition is assumed

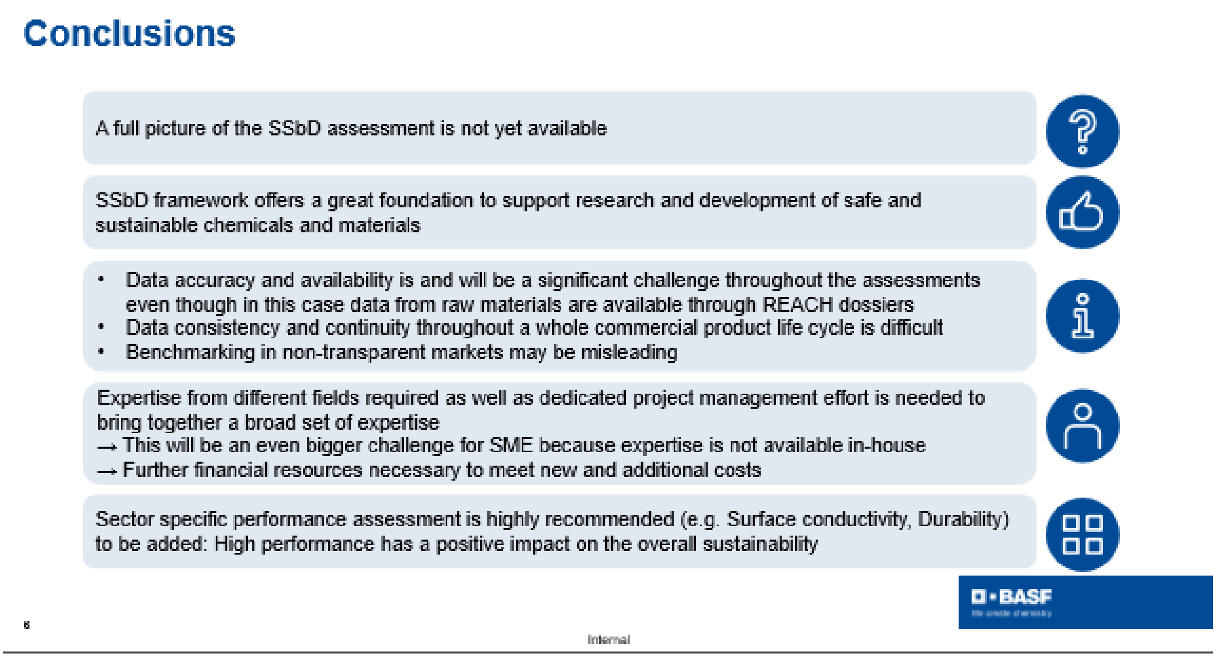
- Life cycle assessment covering a cradle-to-grave approach according to the ISO standards 14040 and 14044 as well as along the lines of the PEF method as benchmark

Challenges & Suggestion

ProScale offers a good feasibility and applicability within the proposed assessment scheme

- ➢ ProScale to be implemented for PEF
- ➢ ProScale for ecotoxicity assessment is currently under development and may be applied in this case

- Data from all components of the material are not available
- PEFCR not fully available for respective product type
- Data accuracy difficult to maintain
  - ➢ Varying data for raw materials throughout the product's life-cycle (e.g. multiple suppliers, production sites)



Conclusions

A full picture of the SSbD assessment is not yet available

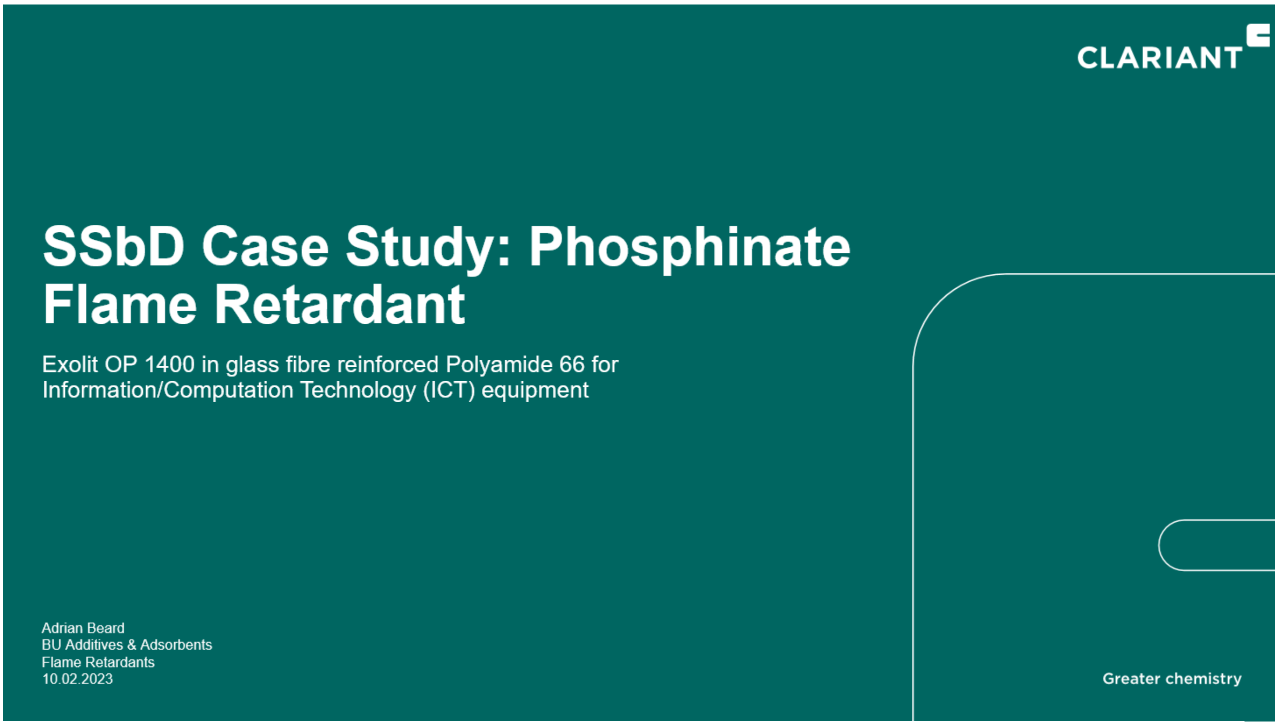
SSbD framework offers a great foundation to support research and development of safe and sustainable chemicals and materials

- Data accuracy and availability is and will be a significant challenge throughout the assessments even though in this case data from raw materials are available through REACH dossiers
- Data consistency and continuity throughout a whole commercial product life cycle is difficult
- Benchmarking in non-transparent markets may be misleading

Expertise from different fields required as well as dedicated project management effort is needed to bring together a broad set of expertise
→ This will be an even bigger challenge for SME because expertise is not available in-house
→ Further financial resources necessary to meet new and additional costs

Sector specific performance assessment is highly recommended (e.g. Surface conductivity, Durability) to be added: High performance has a positive impact on the overall sustainability

Clariant presentation



CLARIANT

SSbD Case Study: Phosphinate Flame Retardant

Exolit OP 1400 in glass fibre reinforced Polyamide 66 for
Information/Computation Technology (ICT) equipment

Adrian Beard
BU Additives & Adsorbents
Flame Retardants
10.02.2023

Greater chemistry

2 SSbD Case Study: Phosphinate Flame Retardant
Adrian Beard, BU Additives & Adsorbents, Flame Retardants, 10.02.2023

Exolit® OP phosphinate based flame retardants – the industry benchmark for halogen free engineering plastics

Non-melting filler like flame retardants,
available as single substance or
in the combination with synergists,
typical dosage 20%

Exolit OP

Polyamides

Polyesters

Thermoplastic Elastomers

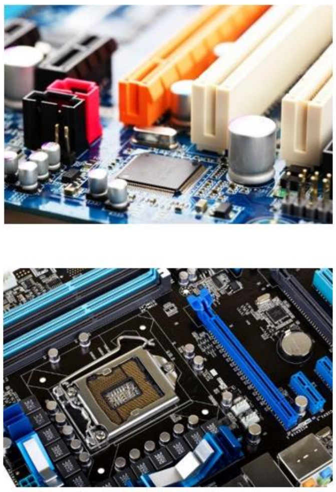
Epoxies, Adhesives,
Textile Coating . . .

The use case: Exolit OP 1400 in PA66 GF in ICT equipment

USB Type C connectors
DDR memory sockets
PCB sockets / connectors

Exolit OP 1400 = blend of phosphinate + synergist

© A. Beard

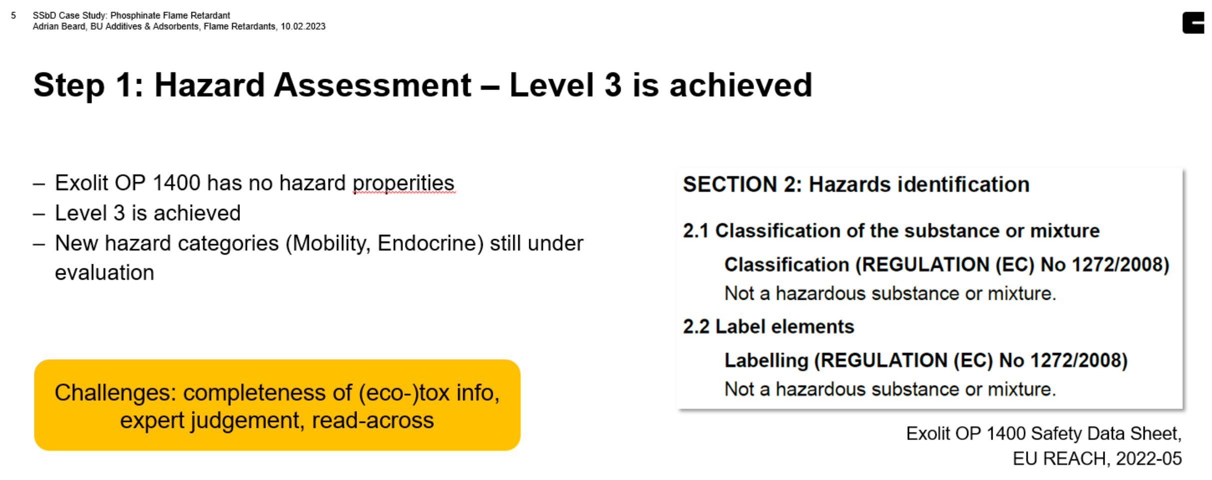


© Shutterstock

The Electronics Value Chain

Raw materials
FR Producer (Clariant)
Compounder
Part Manufacturer
Equipment Manufacturer

Challenges: information flow / confidential business info



5 SSbD Case Study: Phosphinate Flame Retardant
Adrian Beard, BU Additives & Adsorbents, Flame Retardants, 10.02.2023

Step 1: Hazard Assessment – Level 3 is achieved

- Exolit OP 1400 has no hazard properities
- Level 3 is achieved
- New hazard categories (Mobility, Endocrine) still under evaluation

Challenges: completeness of (eco-)tox info, expert judgement, read-across

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)
Not a hazardous substance or mixture.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)
Not a hazardous substance or mixture.

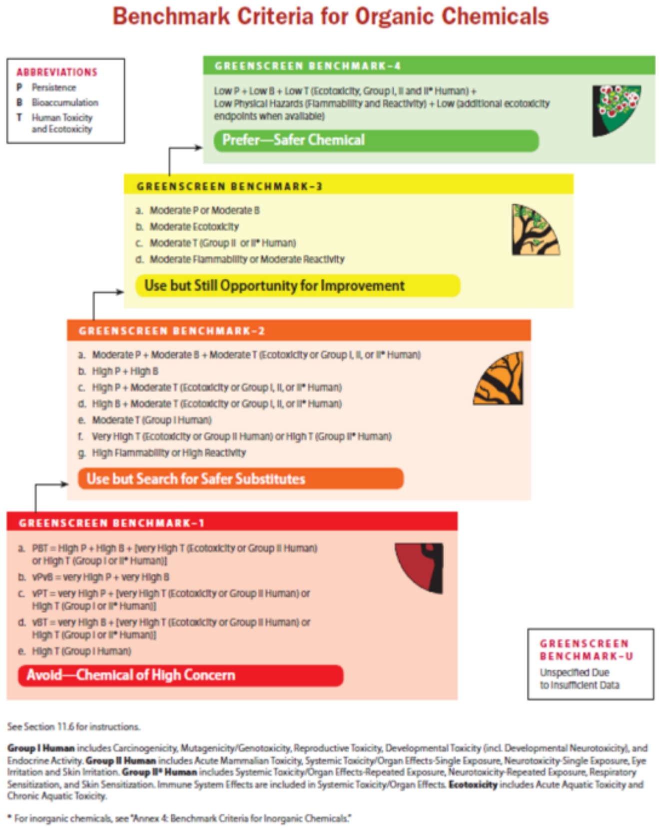
Exolit OP 1400 Safety Data Sheet,
EU REACH, 2022-05

6 SSbD Case Study: Phosphinate Flame Retardant
Adrian Beard, BU Additives & Adsorbents, Flame Retardants, 10.02.2023

Exolit® OP phosphinate flame retardants have a proven environmental and health profile – they also achieve Clariant's EcoTain® label

EU ENFIRO Project

GreenScreen Benchmark 3 for Exolit OP / DEPAL is excellent



Benchmark Criteria for Organic Chemicals

ABBREVIATIONS
P Persistence
B Bioaccumulation
T Human Toxicity and Ecotoxicity

GREENSCREEN BENCHMARK-4

Low P + Low B + Low T (Ecotoxicity, Group I, II and II* Human) + Low Physical Hazards (Flammability and Reactivity) + Low (additional ecotoxicity endpoints when available)

Prefer—Safer Chemical

GREENSCREEN BENCHMARK-3

a. Moderate P or Moderate B
b. Moderate Ecotoxicity
c. Moderate T (Group II or II* Human)
d. Moderate Flammability or Moderate Reactivity

Use but Still Opportunity for Improvement

GREENSCREEN BENCHMARK-2

a. Moderate P + Moderate B + Moderate T (Ecotoxicity or Group I, II, or II* Human)
b. High P + High B
c. High P + Moderate T (Ecotoxicity or Group I, II, or II* Human)
d. High B + Moderate T (Ecotoxicity or Group I, II, or II* Human)
e. Moderate T (Group I Human)
f. Very High T (Ecotoxicity or Group II Human) or High T (Group II* Human)
g. High Flammability or High Reactivity

Use but Search for Safer Substitutes

GREENSCREEN BENCHMARK-1

a. PBT = High P + High B + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]
b. vPvB = very High P + very High B
c. vPT = very High P + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]
d. vBT = very High B + [very High T (Ecotoxicity or Group II Human) or High T (Group I or II* Human)]
e. High T (Group I Human)

Avoid—Chemical of High Concern

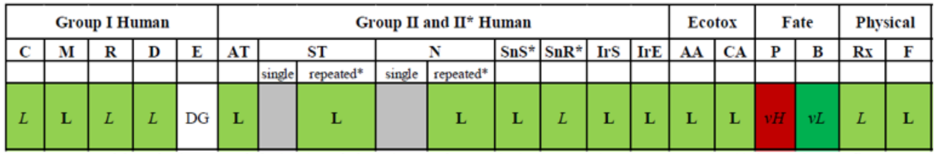
GREENSCREEN BENCHMARK-U
Unspecified Due to Insufficient Data

See Section 11.6 for instructions.

Group I Human includes Carcinogenicity, Mutagenicity/Genotoxicity, Reproductive Toxicity, Developmental Toxicity (incl. Developmental Neurotoxicity), and Endocrine Activity. **Group II Human** includes Acute Mammalian Toxicity, Systemic Toxicity/Organ Effects-Single Exposure, Neurotoxicity-Single Exposure, Eye Irritation and Skin Irritation. **Group II* Human** includes Systemic Toxicity/Organ Effects-Repeated Exposure, Neurotoxicity-Repeated Exposure, Respiratory Sensitization, and Skin Sensitization. Immune System Effects are included in Systemic Toxicity/Organ Effects. **Ecotoxicity** includes Acute Aquatic Toxicity and Chronic Aquatic Toxicity.

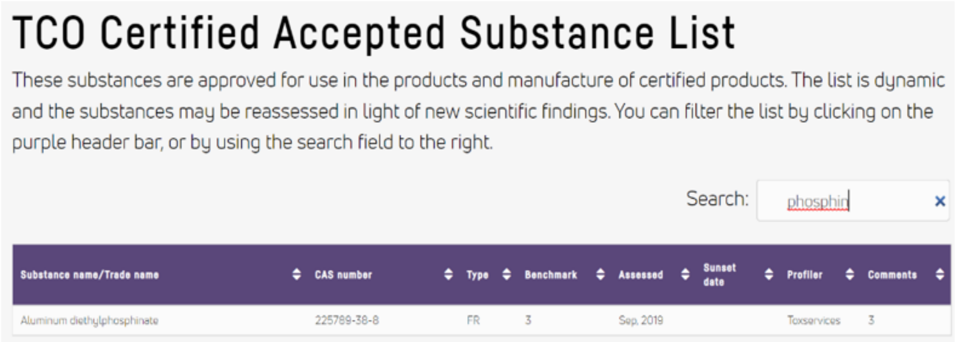
* For inorganic chemicals, see "Annex 4: Benchmark Criteria for Inorganic Chemicals."

Table 1: GreenScreen® Hazard Summary Table for Aluminum Diethylphosphinate



Group I Human					Group II and II* Human									Ecotox		Fate		Physical	
C	M	R	D	E	AT	ST		N		SnS*	SnR*	IrS	IrE	AA	CA	P	B	Rx	F
						single	repeated*	single	repeated*										
L	**L**	*L*	*L*	DG	**L**		**L**		**L**	**L**	*L*	**L**	**L**	**L**	**L**	*vH*	*vL*	*L*	**L**

Note: Hazard levels (Very High (vH), High (H), Moderate (M), Low (L), Very Low (vL)) in *italics* reflect lower confidence in the hazard classification while hazard levels in **BOLD** font reflect higher confidence.



TCO Certified Accepted Substance List

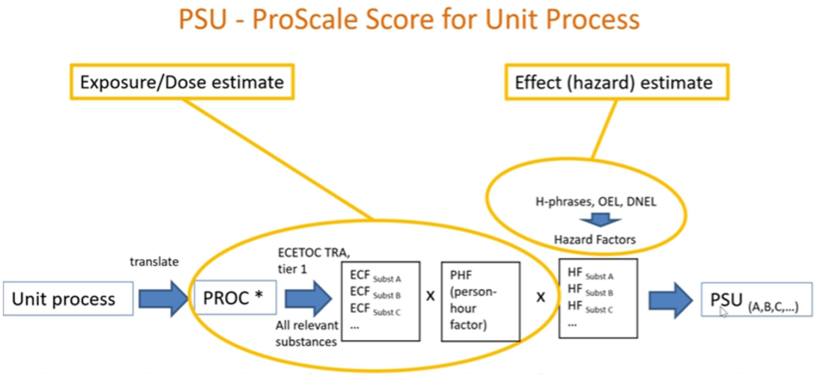
These substances are approved for use in the products and manufacture of certified products. The list is dynamic and the substances may be reassessed in light of new scientific findings. You can filter the list by clicking on the purple header bar, or by using the search field to the right.

Search: phosphin

Substance name/Trade name	CAS number	Type	Benchmark	Assessed	Sunset date	Profiler	Comments
Aluminum diethylphosphinate	225789-38-8	FR	3	Sep. 2019		Toxservices	3

Step 2: Production and Processing – Health & Safety Aspects

- ProScale Assessment:
  - Clariant Processes
    - DEPAL synthesis
    - Synergist synthesis
  - Upstream:
    - P4
    - Intermediate 1
    - Intermediate 2
    - Intermediate 3



PSU - ProScale Score for Unit Process

Exposure/Dose estimate

Effect (hazard) estimate

H-phrases, OEL, DNEL

Hazard Factors

Unit process

translate

PROC *

ECETOC TRA, tier 1

All relevant substances

ECF $_{\text{Subst A}}$
ECF $_{\text{Subst B}}$
ECF $_{\text{Subst C}}$
...

x

PHF (person-hour factor)

x

HF $_{\text{Subst A}}$
HF $_{\text{Subst B}}$
HF $_{\text{Subst C}}$
...

PSU $_{(A,B,C,...)}$

*) Process category (PROC): ECHA guidance on Information Requirements and Chemical Safety Assessment Chapter R.12: Use description
For use and service life processes, different notations than PROC is used

Challenges: process / substance info from suppliers, confidentiality

Step 3: Final Application Phase: Health & Environment

- Under evaluation with Clariant (Eco-)Tox Department

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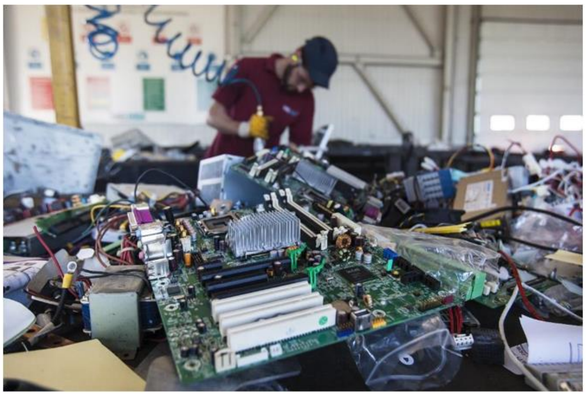


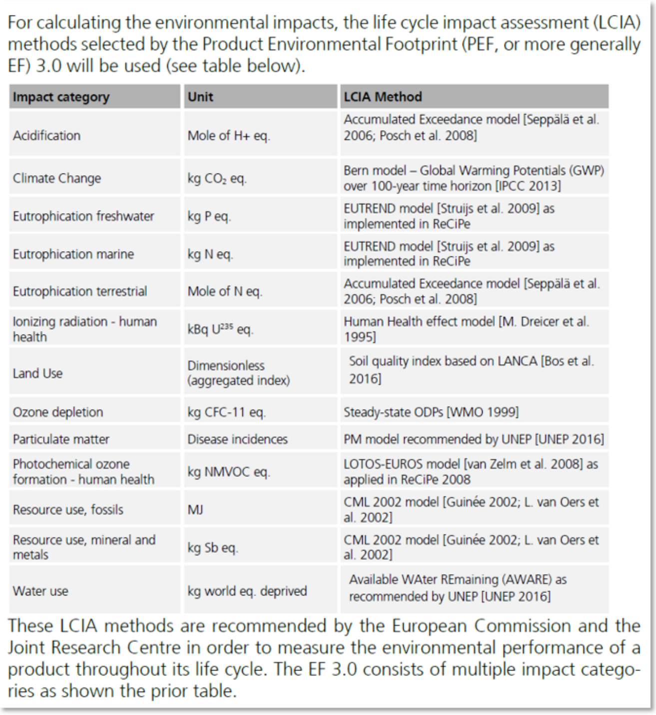
© Shutterstock

Challenge: additional step, not required under REACH

Step 4: Environmental Sustainability Assessment

– LCA being performed by Fraunhofer UMSICHT

Challenges:
process / substance info from suppliers, confidentiality, €€€



For calculating the environmental impacts, the life cycle impact assessment (LCIA) methods selected by the Product Environmental Footprint (PEF, or more generally EF) 3.0 will be used (see table below).

Impact category	Unit	LCIA Method
Acidification	Mole of H+ eq.	Accumulated Exceedance model [Seppälä et al. 2006; Posch et al. 2008]
Climate Change	kg CO_2 eq.	Bern model – Global Warming Potentials (GWP) over 100-year time horizon [IPCC 2013]
Eutrophication freshwater	kg P eq.	EUTREND model [Struijs et al. 2009] as implemented in ReCiPe
Eutrophication marine	kg N eq.	EUTREND model [Struijs et al. 2009] as implemented in ReCiPe
Eutrophication terrestrial	Mole of N eq.	Accumulated Exceedance model [Seppälä et al. 2006; Posch et al. 2008]
Ionizing radiation - human health	kBq U^{235} eq.	Human Health effect model [M. Dreicer et al. 1995]
Land Use	Dimensionless (aggregated index)	Soil quality index based on LANCA [Bos et al. 2016]
Ozone depletion	kg CFC-11 eq.	Steady-state ODPs [WMO 1999]
Particulate matter	Disease incidences	PM model recommended by UNEP [UNEP 2016]
Photochemical ozone formation - human health	kg NMVOC eq.	LOTOS-EUROS model [van Zelm et al. 2008] as applied in ReCiPe 2008
Resource use, fossils	MJ	CML 2002 model [Guinée 2002; L. van Oers et al. 2002]
Resource use, mineral and metals	kg Sb eq.	CML 2002 model [Guinée 2002; L. van Oers et al. 2002]
Water use	kg world eq. deprived	Available WAter REmaining (AWARE) as recommended by UNEP [UNEP 2016]

These LCIA methods are recommended by the European Commission and the Joint Research Centre in order to measure the environmental performance of a product throughout its life cycle. The EF 3.0 consists of multiple impact categories as shown the prior table.

First Learnings from JRC SSbD Approach

1. guidance provides a very broad and comprehensive methodology
2. requires very high efforts (PEF, LCA, €€€)
3. need for screening methods and a tiered approach

Scout → Scope → Execute → Commercialize

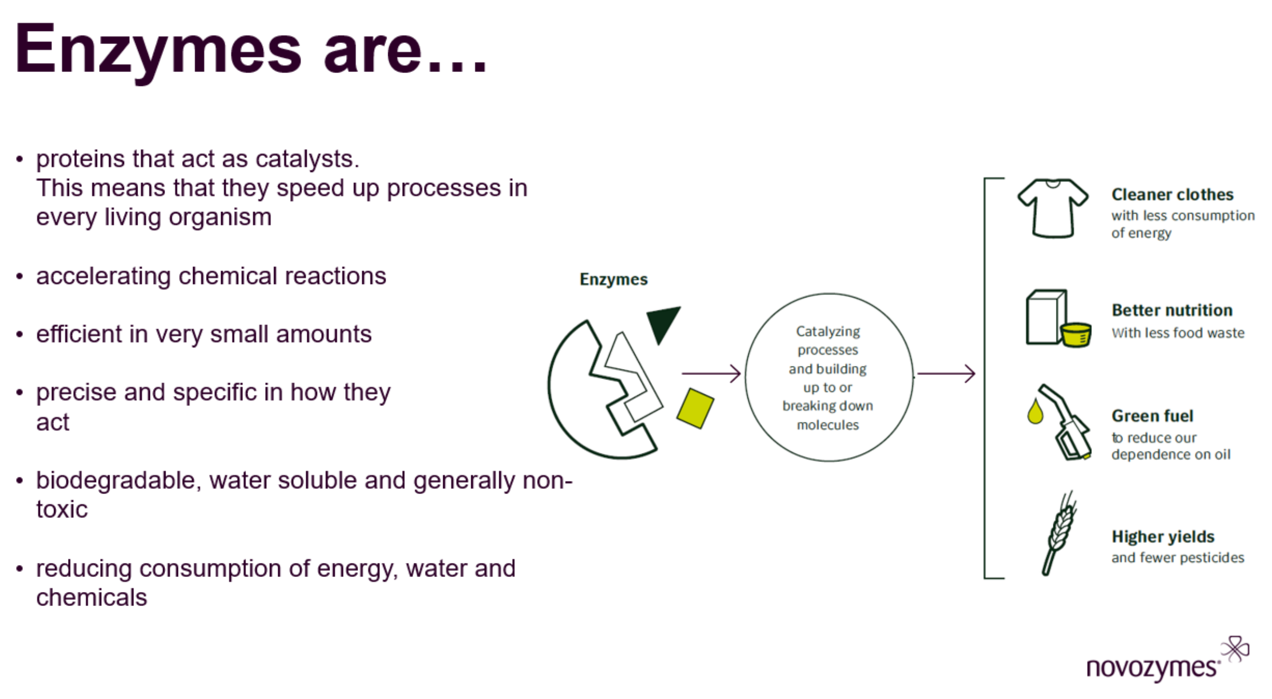
4. when substituting existing products, go for “sustainability hotspots”
   a) raw materials, which have particular hazards
   b) processes with high energy consumption and emissions
   c) life cycle stages with particular issues which need improvement
5. vs. quantification vs. expert judgement (with peer review)
6. also: production processes or raw materials can bring sustainability improvements
7. flame retardants: fire during the life cycle of products?

Clariant Portfolio Management (clariant.com)
WBCSD Portfolio Assessment Platform

Case study 3: Surfactants in textiles
Novozymes

SSbD case study
Scouring of cotton

Katarzyna Cenian, Rie Tsuchiya
February 10, 2023



Enzymes are…

- proteins that act as catalysts. This means that they speed up processes in every living organism
- accelerating chemical reactions
- efficient in very small amounts
- precise and specific in how they act
- biodegradable, water soluble and generally non-toxic
- reducing consumption of energy, water and chemicals

Enzymes

Catalyzing processes and building up to or breaking down molecules

Cleaner clothes
with less consumption of energy

Better nutrition
With less food waste

Green fuel
to reduce our dependence on oil

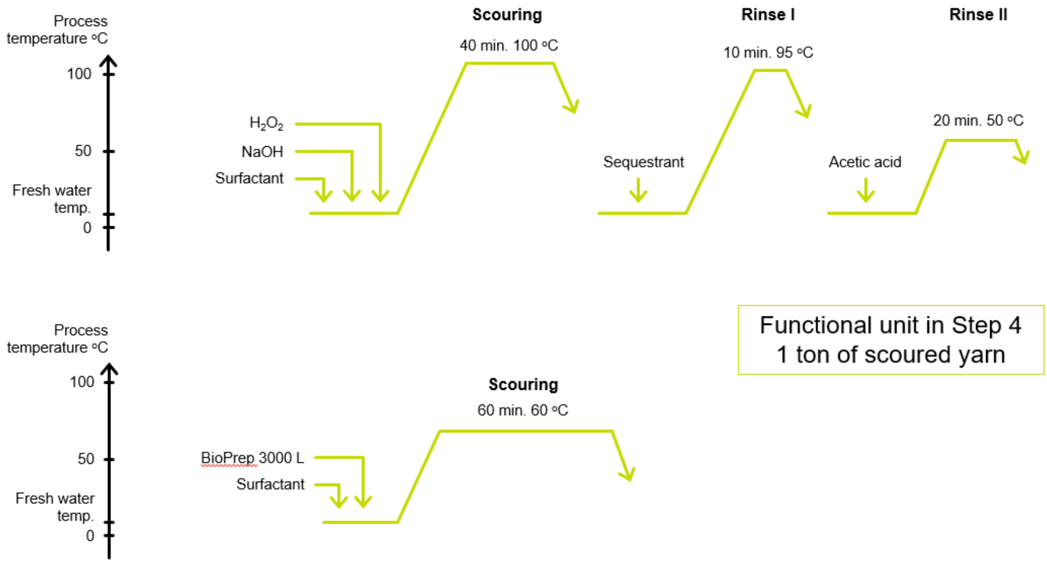
Higher yields
and fewer pesticides

Case study: Scouring of cotton with BioPrep 3000 L

Cotton fibers are covered by a thin layer of wax which needs to be removed prior to dyeing of cotton textiles.

Novozymes **BioPrep 3000 L** is a pectate lyase which degrades pectin - the 'glue' between the cotton fiber and the wax - and **facilitates the removal of wax and other impurities.**

Scouring of dark shade yarn



Conventional scouring

Process temperature °C

100

50

Fresh water temp.

0

H_2O_2

NaOH

Surfactant

Scouring

40 min. 100 °C

Sequestrant

Rinse I

10 min. 95 °C

Acetic acid

Rinse II

20 min. 50 °C

Functional unit in Step 4
1 ton of scoured yarn

Enzymatic scouring

Process temperature °C

100

50

Fresh water temp.

0

BioPrep 3000 L

Surfactant

Scouring

60 min. 60 °C

Step 1 Hazard assessment (Intrinsic properties)

	Pectate lyase
Public name	Lyase, pectate
EC no.	232-766-9
CAS no.	9015-75-2
REACH Registration	Registered
CLP classification	Resp. Sens. 1, H334 (Self classification)
Group definition*	Group A

- Like other proteins, enzymes are only able to cause allergy by inhalation (Type I) = respiratory sensitizer
- Enzymes are neither stronger nor weaker than allergens commonly found in nature
- Pectate lyase is classified as Respiratory Sensitizers Category 1 in REACH dossier

The JRC Technical Report on SSbD proposes that the most harmful substances should be used for cut-off criteria for SSbD.

Given our industry long-standing experience in ensuring enzymes' safety, their positive environmental impact and their biological profiles, we proceeded with the further steps of the JRC framework despite pectate lyase belonging to Group A.

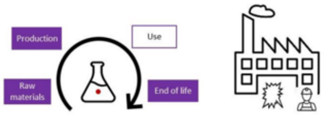
This example illustrates the limitations of a hazard-based cutoff for safe and sustainable chemicals and products.

Learning

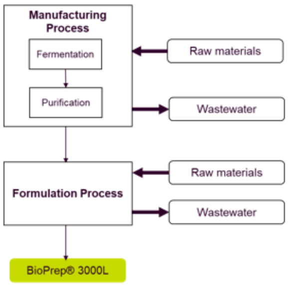
- The cut-off criterion **prevents enzyme-based innovation from contributing to the circular economy and the green transition**
- QSAR cannot be used for substances like enzymes. If substances are new and QSAR cannot be used, Step 1 would require toxicological studies to identify hazards.

novozymes

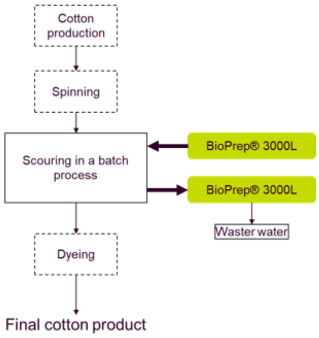
Step 2 Human health and safety aspects of production and processing



- Process can be identified with descriptors used in REACH CSR.
- Risk Characterisation Ratio (RCR) can be used for scoring. For enzymes, Derived Minimal Exposure Level (**DMEL**) 60ng/m^3 for workers
- Exposure assessments were done with actual measurements



Manufacturing and formulation process for BioPrep 3000L



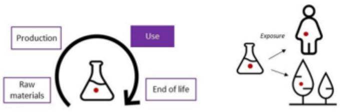
Scouring process with BioPrep 3000L

Learning

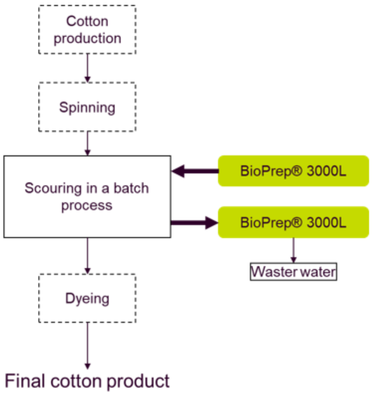
- **DMELs**: There is **no animal model** for respiratory sensitizers. **DMELs for enzymes** are derived based on **actual measurements of enzyme exposures and medical surveillance** generated by the enzyme and detergent industries for **over 50 years.**
- **Exposure assessment:** Tier I tools such as ECETOC TRA cannot be used for respiratory sensitizers. **Currently actual measurements is only way to assess enzyme exposures.** It would be optimal if IT tool for such substances is developed.

novozymes

Step 3 Human health and environmental aspects of the final application



- The case study is process improvement. There is no impact on final cotton product.



Learning

- Consumers get cotton products /cloths with the same quality either with the conventional scouring or the enzymatic scouring. Thereby, there is no Step 3 in this case study.
- How Step 3 should be documented in this case?

Step 4 Environmental sustainability assessment

Background of the study

Novozymes is new to PEF, but we have +15 years experience with LCA, following ISO 14040/44

Inventory of our product was (almost) readily available in LCA software

- ❯ No feedback on data collection, which can be a challenging and time-consuming step

Lack of EF-compliant secondary datasets

- ❯ No feedback on datasets coverage, quality etc.

Step 4 Environmental sustainability assessment

Main learnings

EF 3.0 impact assessment method lacks factors for direct emissions of pectate lyase (or any other enzyme) to environment

- Human toxicity, non-carcinogenic and freshwater ecotoxicity could not be assessed

The underlying toxicity model – USEtox – may not be suitable to derive factors for enzymes

- No immediate solution to toxicity assessment

Lack of a procedure/dataset for modelling treatment of specific composition of wastewater

- Simplified end of life, not reflecting high degradation rate of enzymes

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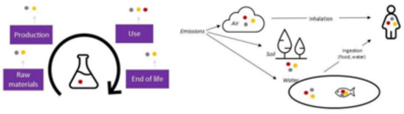
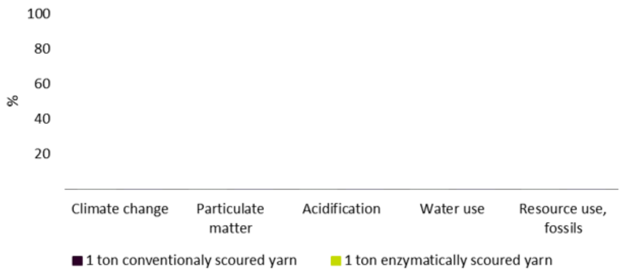
Step 4 Environmental sustainability assessment

Summary of PEF results



- Five most relevant impact categories
- Enzymatic scouring has approx. **60% lower impact** than conventional process
- The reduction is mainly driven by **decrease in steam and water** consumption



Summary and Proposals

Summary

Step 1: Pectate lyase – an enzyme in BioPrep 3000L is respiratory sensitizer category 1

Step 2: Risk Characterization Ratio (RCR) used in REACH CSR can be applied to BioPrep 3000 L.

Step 3: No assessment was made. The case study is process improvement and there is no impact on consumer products (cotton products/cloths).

Step 4: Enzymatic scouring has lower environmental impact for all impact categories that were covered

Proposals

Step 1: If the hazard-based approach in the cut-off criteria under Step 1 is applied to enzymes, it would push innovation against the objectives of the European Green Deal and the Chemicals Strategy for Sustainability, which aim at increasing the use of bio-based alternatives to synthetic chemicals and Circular Economy.

Step 4: Toxicity of enzymes cannot be assessed with current version of PEF and USEtox. Further development or alternative methods are needed.

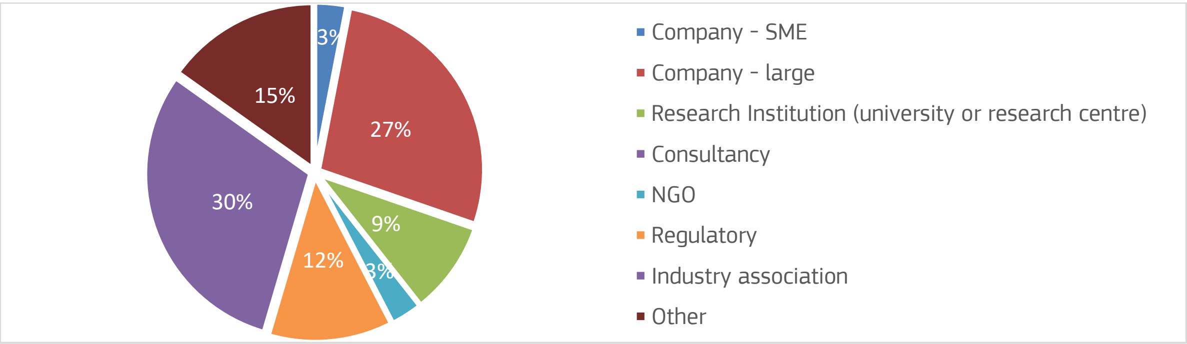
Annex 12. Results from *“3rd Stakeholder workshop – Survey on the SSbD framework”*

The present annex shows the results obtained from the survey launched after the 3rd stakeholder workshop, during the entire period of the open consultation. The goal of the survey was to capture information about the challenges and actions considered by stakeholders as most relevant towards an operationalisation of the framework. Below there are the details for the main questions. At the end of the annex, the questions of the survey are reported.

What kind of organisation do you represent?

As shown in Figure A 29, stakeholders that answered to the survey are mostly Industry associations and large companies. 0% from consultancy and only 3% of SMEs answered to the survey. These results suggest the need of a higher involvement both of SMEs and consultancy for their crucial role in the future regarding the SSbD implementation. Consultancy might represent an important resource for boosting expertise, and SMEs might encounter additional challenges compared to large companies that need to be collected and taken into account.

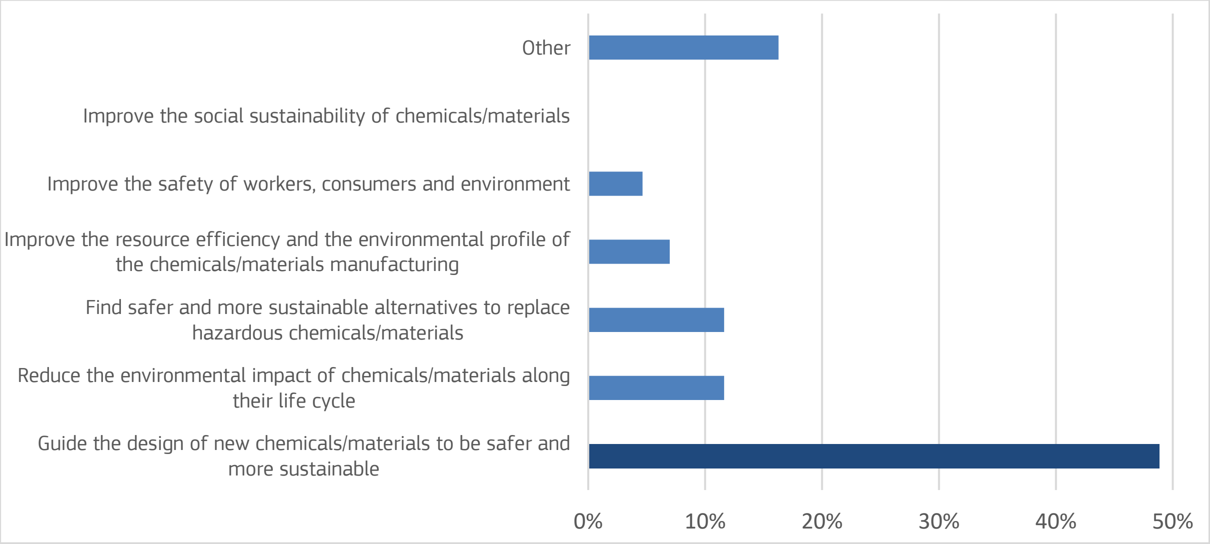
Figure A 29. Distribution of the organizations that answered to the survey



In your opinion, which is the most beneficial application of the Safe and Sustainable by Re-design (SSbD) framework?

The results shown in Figure A 30 outlines that there is a quite common view of the most beneficial application of the SSbD among stakeholders which is the *“guide the re-design of new chemicals/materials to be safer and more sustainable”*. In addition, 60% of stakeholders that answered *“others”* stated *“Harmonisation of safety and sustainability assessments”* as the most beneficial application of the SSbD framework. Both answers suggest the need of an approach able to couple safety and sustainability aspects toward a guidance for chemicals and materials re-design.

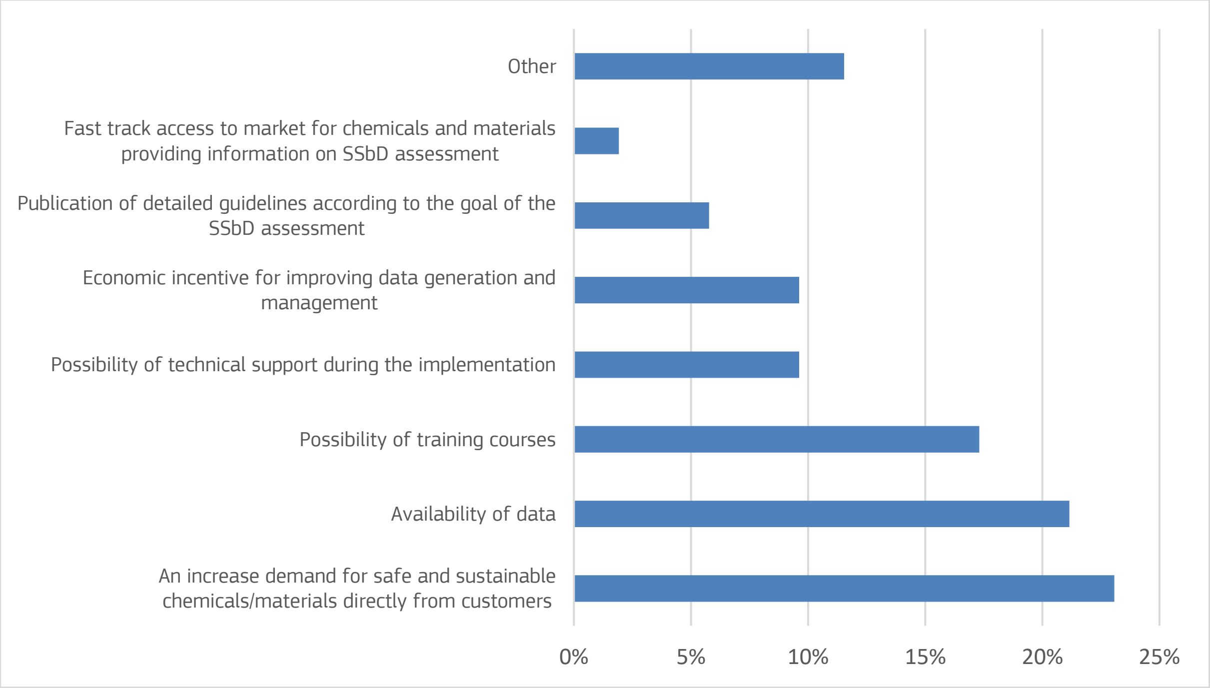
Figure A 30. The most beneficial application of the SSbD framework according to stakeholders’ answers



Which of the following would encourage you to implement the SSbD framework?

There is not a common view on factors that would encourage the implementation of the SSbD framework. As shown in Figure A 31, the majority of stakeholders would be encouraged by the *"increase demand for safe and sustainable chemicals/materials directly from customers"*. This implies the necessity of a robust communication between suppliers and customers along the value chain of products in order to support innovation towards SSbD. The necessity of a robust communication is also raised by the high percentage of answers to the *"availability of data"*. Together with trainings and technical support, the creation of cooperation along the value chains of products has a key role in aiding the implementation of the SSbD framework.

Figure A 31. Factors that would encourage the implementation of the SSbD framework



How important are the following challenges regarding the SSbD assessment?

This question aimed at capturing the most relevant challenges encountered during the development of the case study, from the stakeholders' perspective. Four levels of importance plus *"I don't know"* were considered as possible answers. Collecting all the answers, Figure A 32 shows the final results, which allowed to identify the following three most important challenges according to stakeholders:

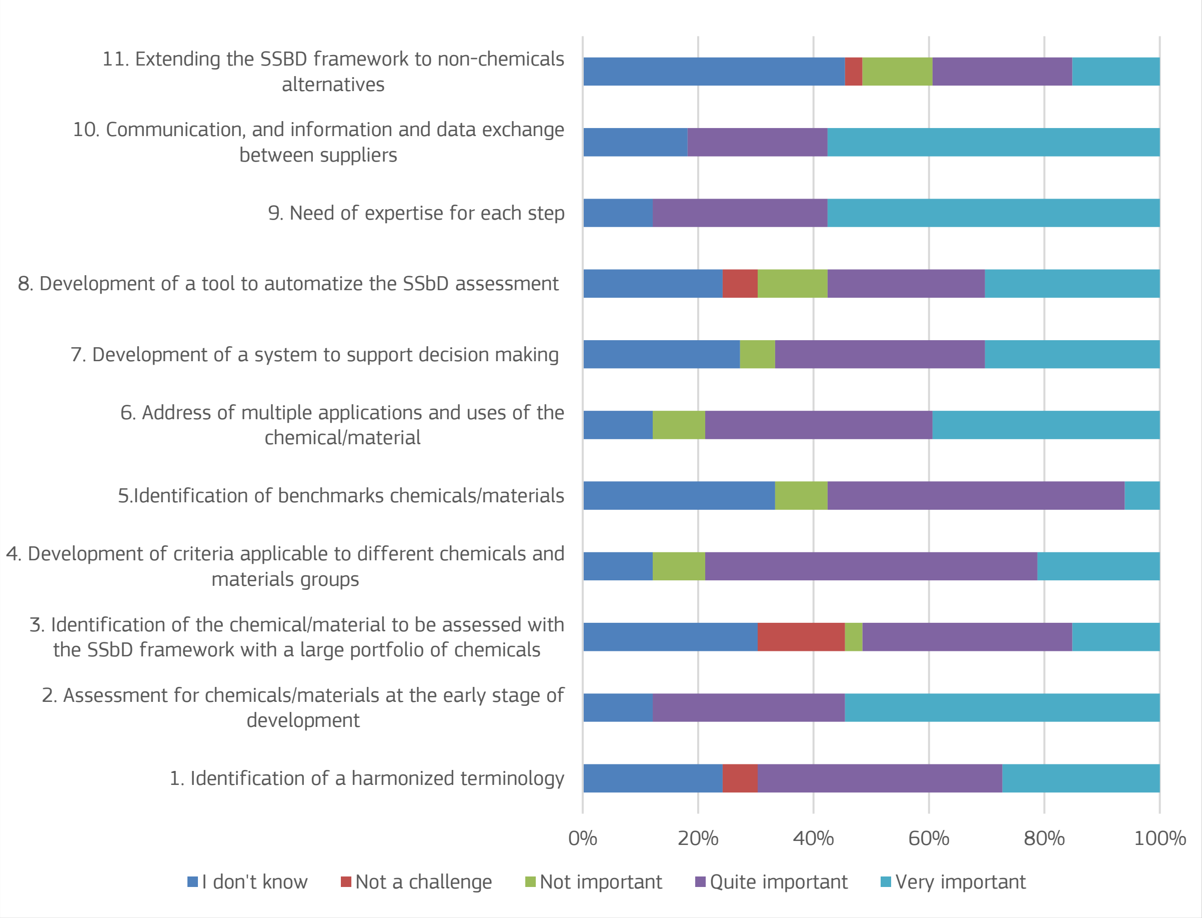
- 2. Assessment for chemicals/materials at the early stage of development (87% answered *"very important"* and *"quite important"*)
- 9. Need of expertise for each step (87% answered *"very important"* and *"quite important"*)
- 10. Communication, information and data exchange between suppliers (81% answered *"very important"* and *"quite important"*)

The three challenges might involve the three main actors for the implementation of the SSbD. Challenge 2 mostly involves researchers to introduce guidelines to support the SSbD assessment throughout the chemical/material development. Challenge 9 mostly might involve regulators and consultancy in boosting the expertise for the implementation of the SSbD framework. Finally, challenge 10 needs a huge effort of industries in creating communication and exchange along the entire supply chain.

Additional relevant challenges to be addressed in the future revealed through the survey are:

- 4. Development of criteria applicable to different chemicals and materials groups
- 6. Address of multiple applications and uses of the chemical/material

Figure A 32. Mapping of the importance of the listed challenges according to stakeholders.



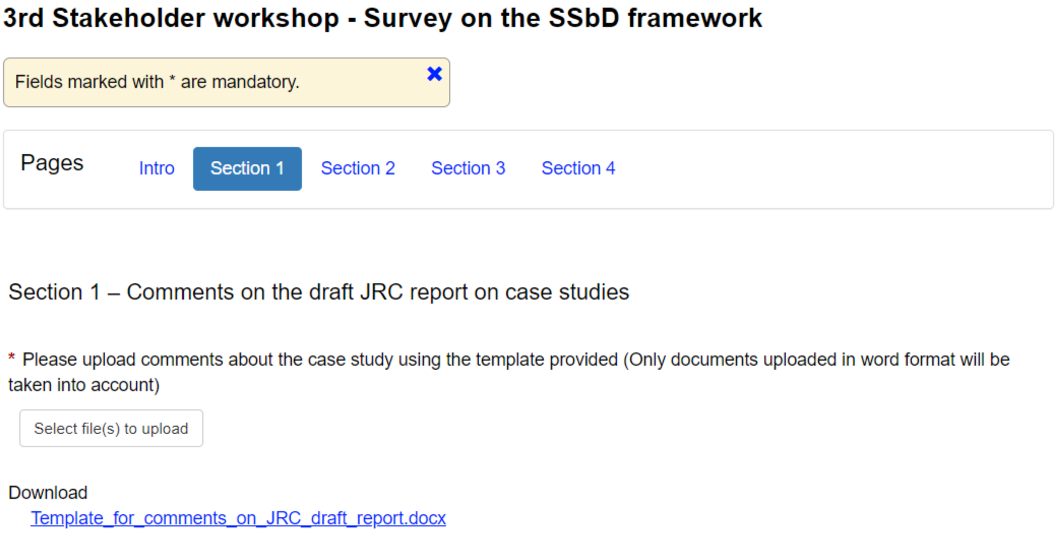
Do you think there are any additional general challenges?

This open question allowed stakeholders to express their general opinion on additional challenges that might be encountered for the implementation of the SSbD framework. The list below summarizes the main additional challenges that were raised from stakeholders.

- Absolute sustainability
- Alignment with other initiatives
- Applicability in the framework (Step 5)
- Appropriate system for the decision making
- Communication to stakeholders
- Cut-off criteria
- Data availability, quality and uncertainty
- Evaluation methodology and criteria definition for the scoring
- Expertise
- Implementation costs
- Multiple uses
- QSAR
- SSbD assessment guidance
- Terminology
- Tiered approach
- Tools
- Use phase definition

Hereafter, the questions of the survey are reported from Figure A 33 to Figure A 38. The survey was split in 4 sections: Section 1 to upload the comments on the draft of the present JRC Technical Report on case studies, Section 2 to collect feedback via the survey, Section 3 to provide suggestions regarding the Reporting Template, and Section 4 to upload any additional supporting documents.

Figure A 33. Survey on the 3rd Stakeholder Workshop. Section 1



3rd Stakeholder workshop - Survey on the SSbD framework

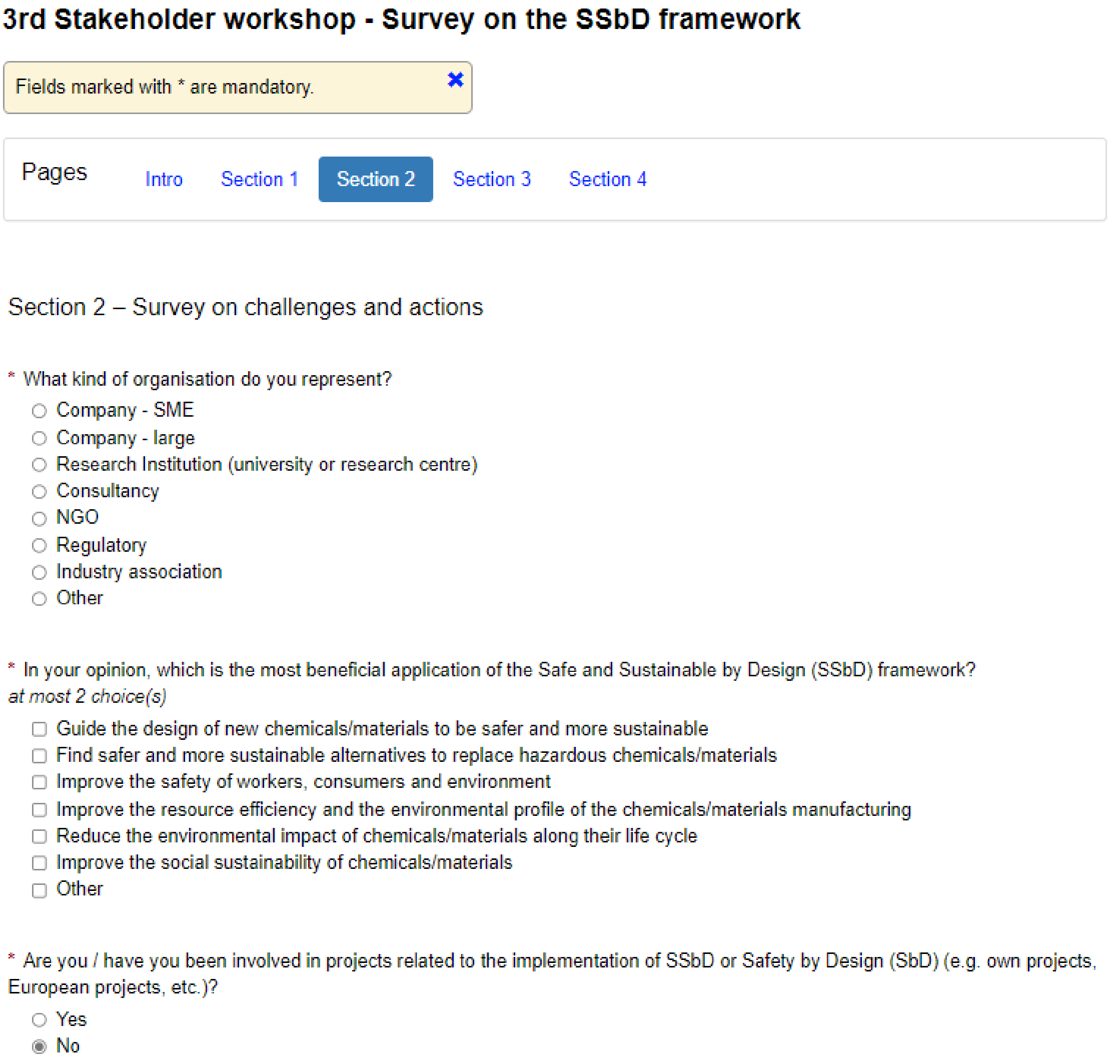
Fields marked with * are mandatory.

Section 1 – Comments on the draft JRC report on case studies

* Please upload comments about the case study using the template provided (Only documents uploaded in word format will be taken into account)

Download
Template_for_comments_on_JRC_draft_report.docx

Figure A 34. Survey on the 3rd Stakeholder Workshop. Section 2



3rd Stakeholder workshop - Survey on the SSbD framework

Fields marked with * are mandatory.

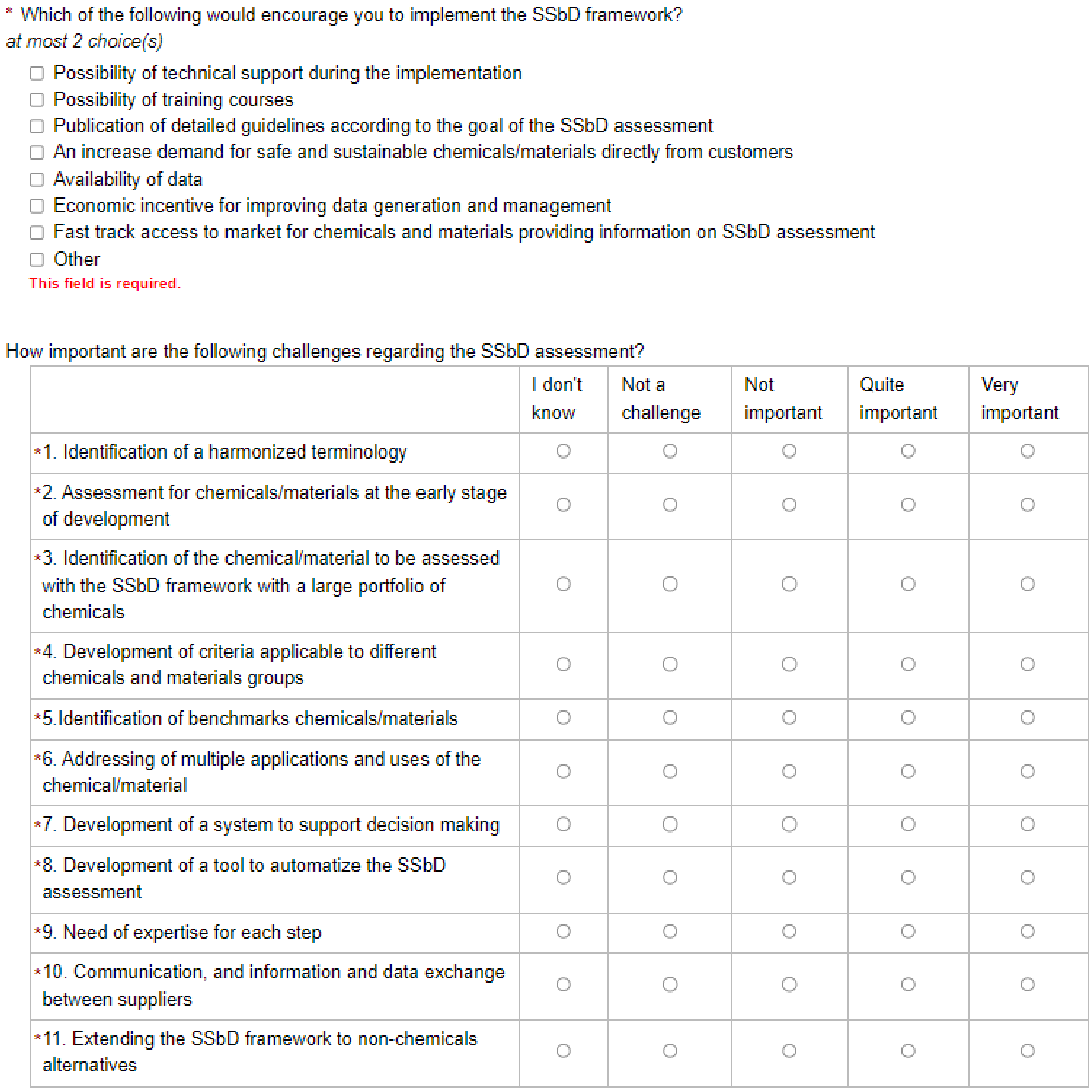
Section 2 – Survey on challenges and actions

* What kind of organisation do you represent?
- ○ Company - SME
- ○ Company - large
- ○ Research Institution (university or research centre)
- ○ Consultancy
- ○ NGO
- ○ Regulatory
- ○ Industry association
- ○ Other

* In your opinion, which is the most beneficial application of the Safe and Sustainable by Design (SSbD) framework?
at most 2 choice(s)
- ☐ Guide the design of new chemicals/materials to be safer and more sustainable
- ☐ Find safer and more sustainable alternatives to replace hazardous chemicals/materials
- ☐ Improve the safety of workers, consumers and environment
- ☐ Improve the resource efficiency and the environmental profile of the chemicals/materials manufacturing
- ☐ Reduce the environmental impact of chemicals/materials along their life cycle
- ☐ Improve the social sustainability of chemicals/materials
- ☐ Other

* Are you / have you been involved in projects related to the implementation of SSbD or Safety by Design (SbD) (e.g. own projects, European projects, etc.)?
- ○ Yes
- ● No

Figure A 35. Survey on the 3rd Stakeholder Workshop. Section 2 - continue



* Which of the following would encourage you to implement the SSbD framework?
at most 2 choice(s)

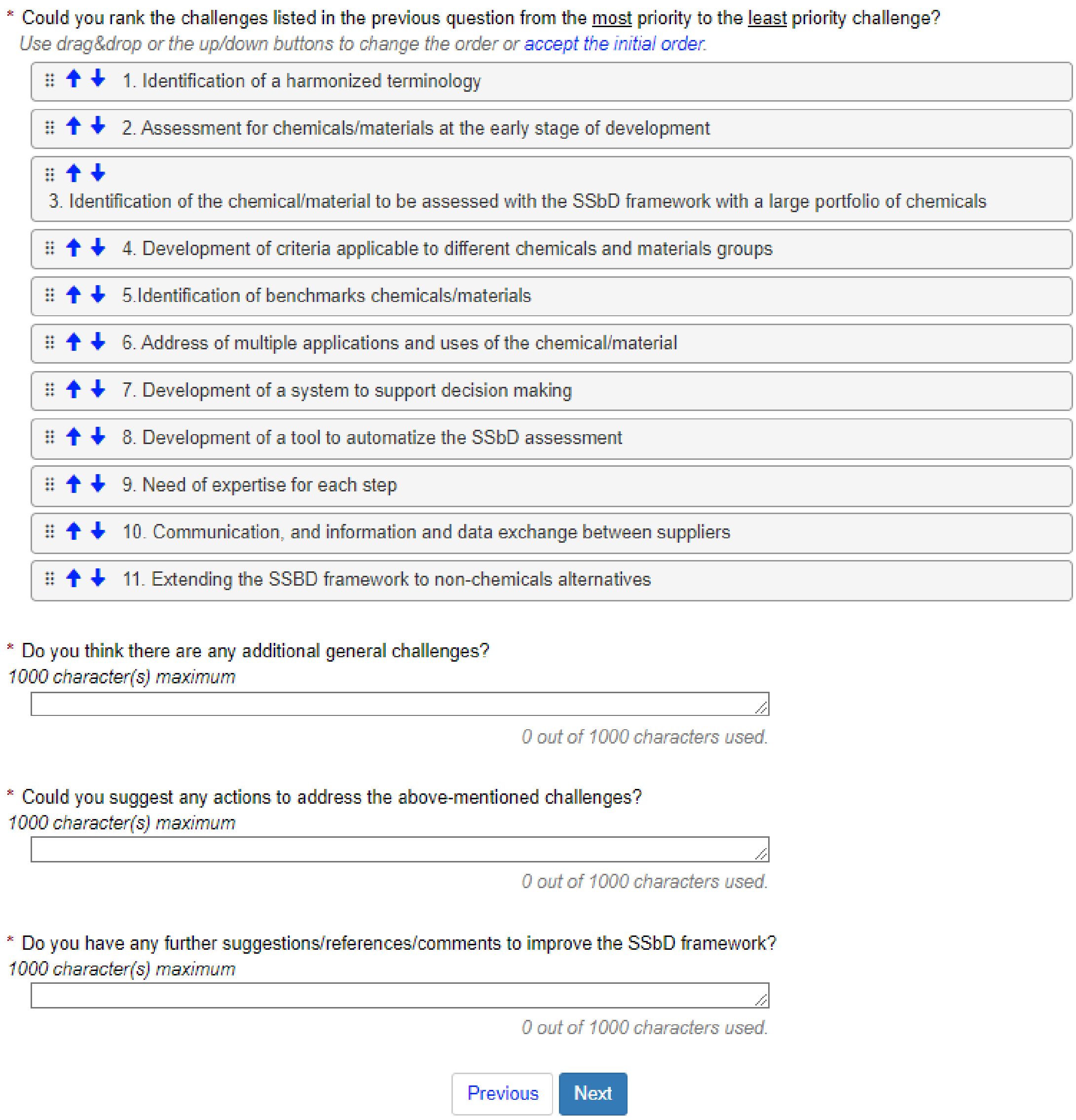
- ☐ Possibility of technical support during the implementation
- ☐ Possibility of training courses
- ☐ Publication of detailed guidelines according to the goal of the SSbD assessment
- ☐ An increase demand for safe and sustainable chemicals/materials directly from customers
- ☐ Availability of data
- ☐ Economic incentive for improving data generation and management
- ☐ Fast track access to market for chemicals and materials providing information on SSbD assessment
- ☐ Other

This field is required.

How important are the following challenges regarding the SSbD assessment?

	I don't know	Not a challenge	Not important	Quite important	Very important
*1. Identification of a harmonized terminology	○	○	○	○	○
*2. Assessment for chemicals/materials at the early stage of development	○	○	○	○	○
*3. Identification of the chemical/material to be assessed with the SSbD framework with a large portfolio of chemicals	○	○	○	○	○
*4. Development of criteria applicable to different chemicals and materials groups	○	○	○	○	○
*5.Identification of benchmarks chemicals/materials	○	○	○	○	○
*6. Addressing of multiple applications and uses of the chemical/material	○	○	○	○	○
*7. Development of a system to support decision making	○	○	○	○	○
*8. Development of a tool to automatize the SSbD assessment	○	○	○	○	○
*9. Need of expertise for each step	○	○	○	○	○
*10. Communication, and information and data exchange between suppliers	○	○	○	○	○
*11. Extending the SSbD framework to non-chemicals alternatives	○	○	○	○	○

Figure A 36. Survey on the 3rd Stakeholder Workshop. Section 2 - continue



* Could you rank the challenges listed in the previous question from the most priority to the least priority challenge?

Use drag&drop or the up/down buttons to change the order or accept the initial order.

1. Identification of a harmonized terminology
2. Assessment for chemicals/materials at the early stage of development
3. Identification of the chemical/material to be assessed with the SSbD framework with a large portfolio of chemicals
4. Development of criteria applicable to different chemicals and materials groups
5. Identification of benchmarks chemicals/materials
6. Address of multiple applications and uses of the chemical/material
7. Development of a system to support decision making
8. Development of a tool to automatize the SSbD assessment
9. Need of expertise for each step
10. Communication, and information and data exchange between suppliers
11. Extending the SSBD framework to non-chemicals alternatives

* Do you think there are any additional general challenges?

1000 character(s) maximum

0 out of 1000 characters used.

* Could you suggest any actions to address the above-mentioned challenges?

1000 character(s) maximum

0 out of 1000 characters used.

* Do you have any further suggestions/references/comments to improve the SSbD framework?

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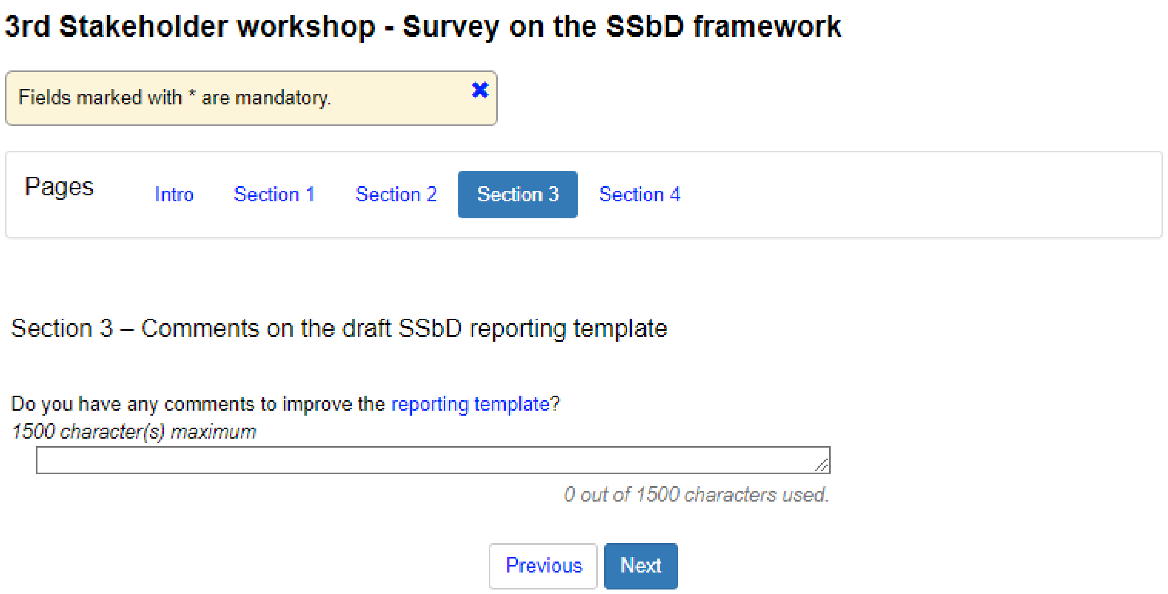
0 out of 1000 characters used.

Figure A 37. Survey on the 3rd Stakeholder Workshop. Section 3



3rd Stakeholder workshop - Survey on the SSbD framework

Fields marked with * are mandatory.

Section 3 – Comments on the draft SSbD reporting template

Do you have any comments to improve the reporting template?

1500 character(s) maximum

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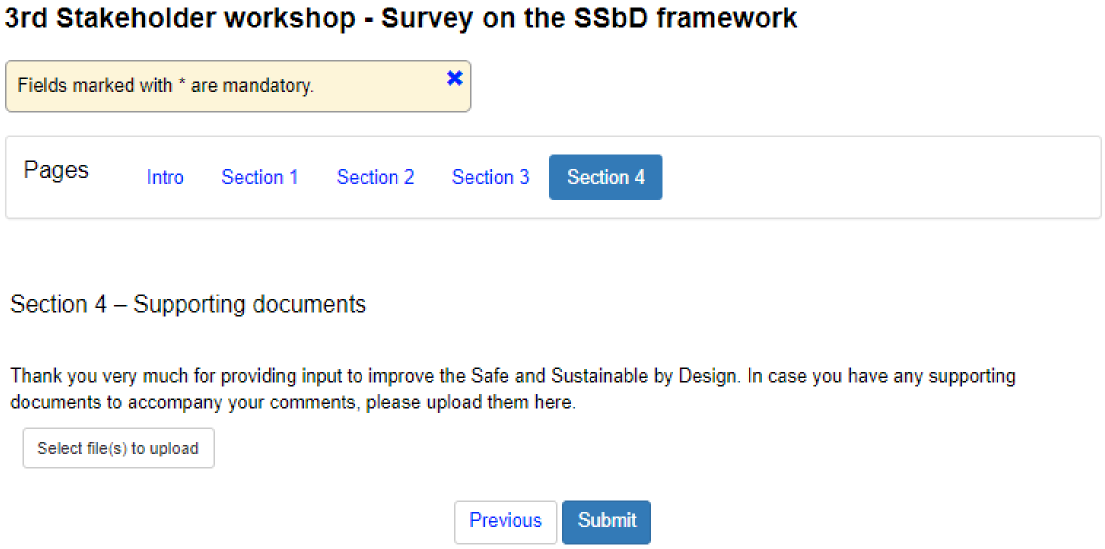
Figure A 38. Survey on the 3rd Stakeholder Workshop. Section 4



3rd Stakeholder workshop - Survey on the SSbD framework

Fields marked with * are mandatory.

Section 4 – Supporting documents

Thank you very much for providing input to improve the Safe and Sustainable by Design. In case you have any supporting documents to accompany your comments, please upload them here.

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