Safe and Sustainable by Design chemicals and materials - Methodological Guidance

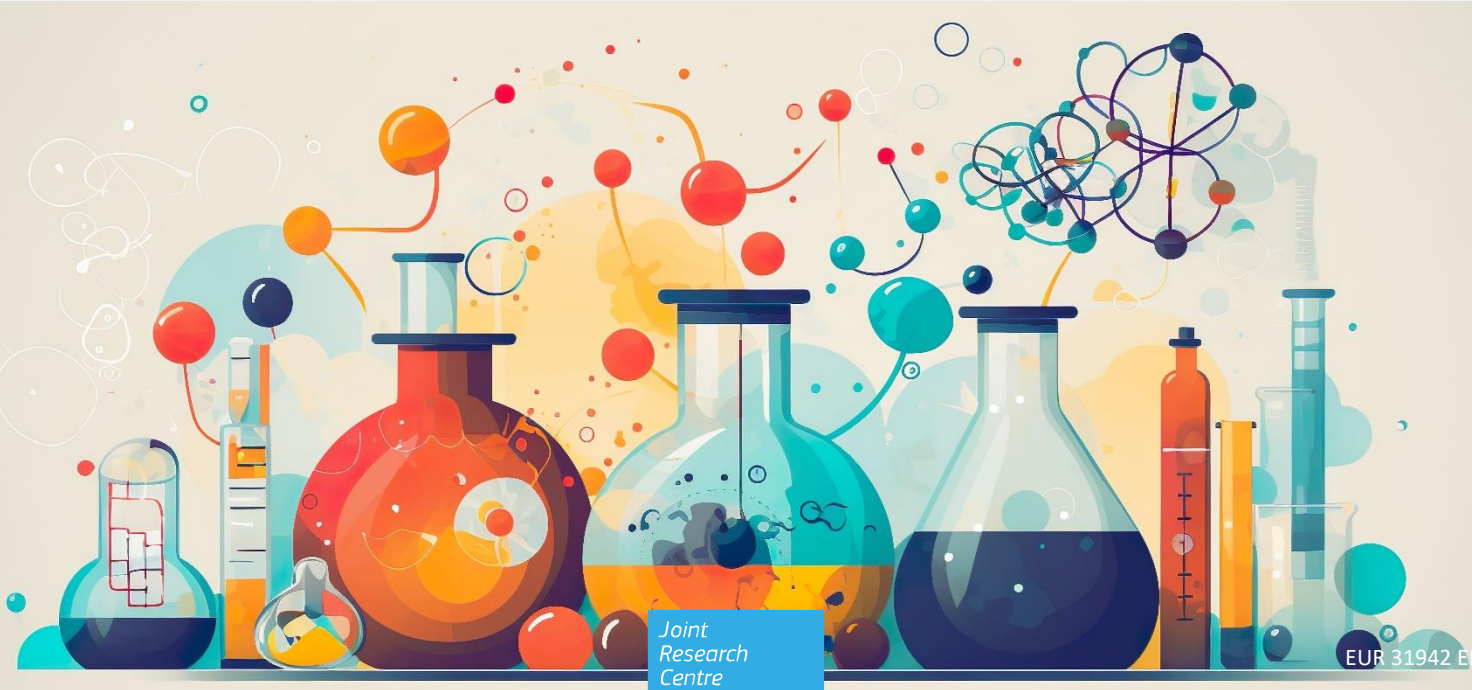
ISSN 1831-9424

European Commission

Safe and Sustainable by Design chemicals and materials - Methodological Guidance

Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H., Sala, S.

2024



Joint Research Centre

EUR 31942 EN

Contact information
Name: Serenella Sala
Address: Via E. Fermi, 2417, Ispra (VA), Italy
Email: Serenella.Sala@ec.europa.eu
Tel.: 0039 0332786417

EU Science Hub
https://joint-research-centre.ec.europa.eu

JRC138035

EUR 31942 EN

PDF ISBN 978-92-68-16357-3 ISSN 1831-9424 doi:10.2760/28450 KJ-NA-31-942-EN-N

Luxembourg: Publications Office of the European Union, 2024

How to cite this report: European Commission, Joint Research Centre, Abbate, E., Garmendia Aguirre, I., Bracalente, G., Mancini, L., Tosches, D., Rasmussen, K., Bennett, M.J., Rauscher, H. and Sala, S.*, Safe and Sustainable by Design chemicals and materials - Methodological Guidance*, Publications Office of the European Union, Luxembourg, 2024, https://data.europa.eu/doi/10.2760/28450, JRC138035.

Contents

Abstract

This Methodological Guidance clarifies some aspects of the voluntary application of the 'safe and sustainable by design' (SSbD) framework for chemicals and materials. It combines the disciplines of "Risk Assessment" (RA) and "Sustainability Assessment" (SA), which have different methodologies, framing and terminology. This Methodological Guidance explains the rationale of the framework and replies to the feedback collected during several stakeholder consultations, which have contributed to its progressive refinement. It furthermore presents a method for scoping analysis and discusses why it is important to correctly frame the subsequent SSbD assessment. Following on, thematic chapters specifically address aspects of the two domains of the framework: safety assessment and environmental sustainability assessment, and also address socio-economic assessment.

Acknowledgements

The authors would like to thank Grazia Maria Cappucci for the input to the Scoping analysis, Jorge Garcia Cristobal for the input to the Frequently Asked Questions (FAQs), Andrea Carbotti and Paivi Sund for the support with graphic layout of the whole document and Birgit Sokull-Klüttgen for supporting the revision and the discussion.

Authors

Elisabetta Abbate, Irantzu Garmendia Aguirre, Giulio Bracalente, Lucia Mancini, Davide Tosches*, Kirsten Rasmussen, Michael Bennett, Hubert Rauscher, Serenella Sala.

*currently Politecnico di Torino, Italy

Executive summary

Policy context

With the European Green Deal (European Commission, 2019) the European Commission (EC) aims to transform the European Union's (EU) economy to support a more sustainable future and to implement the United Nations' agenda 2030. Among the objectives of the Green Deal is the Zero Pollution Ambition (European Commission, 2021b). To achieve this goal, a set of actions were outlined in the Chemicals Strategy for Sustainability (CSS) (European Commission, 2020). Specifically, within the CSS action 2.1 - Innovating for safe and sustainable EU chemicals, sub-action 2.1.1 aims at promoting 'safe and sustainable by design' chemicals, while sub-action 2.1.2 aims at achieving safe products and non-toxic material cycles.

In 2022, the EC adopted a Recommendation establishing a European assessment framework for SSbD chemicals and materials to support the implementation of the CSS (EC, 2022a). The scientific-technical basis for the Recommendation, i.e., the SSbD framework, was developed by the EC's Joint Research Centre (JRC) (Caldeira et al., 2022a).

Main findings

The Methodological Guidance (henceforth 'the Guidance') clarifies certain aspects of the application of the SSbD framework, bearing in mind that the latter is a voluntary approach combining several disciplines, primarily risk assessment and sustainability assessment, which differ, among others, in established methodologies, framing and terminology. The Guidance is intended for professionals wishing to apply the SSbD framework in the research and innovation (R&I) area to develop new chemicals, materials and/or products, including developers of funding programmes supporting such innovations.

Related and future JRC work

The JRC has been involved in assessing the safety of chemicals since the early 1990s, and in addition has developed methodologies for sustainability assessment for decades.

With the European Green Deal and the CSS, the JRC was asked to develop a framework that could help to evaluate the level of safety and sustainability for chemicals and materials. This framework (Caldeira. et al., 2022a) was developed based on a review of other existing frameworks (Caldeira et al., 2022b), and was integrated into the EC Recommendation establishing a European assessment framework for the 'safe and sustainable by design' of chemicals and materials to support the implementation of the CSS (European Commission, 2022a). The JRC tested the framework by performing a complete case study (Caldeira et al., 2023), and assisting industry stakeholders in performing two additional case studies. The SSbD framework has been intensely promoted and consulted upon. Based on the feedback solicited and received, including from the first reporting period in May-June 2023 and expected from the second reporting period May-August 2024, it is planned for the JRC to update the framework in 2025.

Quick guide

The structure of the Guidance follows the overall SSbD structure. Section 2 presents the overall framework in a nutshell, followed by Section 3 which presents the scoping analysis and discusses why it is important to correctly frame the subsequent SSbD assessment. Following on, thematic chapters specifically address aspects of the two domains of the framework: safety assessment and environmental sustainability assessment and finally also discuss socio-economic assessment.

1 Introduction

This Guidance is intended for **professionals wishing to apply the SSbD framework**. This includes innovators working in the research and innovation (R&I) areas and that develop new chemicals, materials, processes, and/or products. In addition, it is intended also for assessors that take care of the safety and sustainability performance of these developments. For that reason, the guidance refers to these two important actors in the implementation of the framework, and when it refers to either of the two it uses the term "practitioner".

Stakeholders have indicated the main challenge regarding the implementation of the SSbD framework concerns difficulties in implementing the steps of the assessment along the innovation process. Thus, the main goal of the Guidance is **to provide explanations and examples, and to present possible actions to address this challenge.** The general assumption is that the reader has a detailed familiarity with the Commission Recommendation (European Commission, 2022a), the contents of the framework (Caldeira et al., 2022a) and knowledge on design, safety and sustainability. Therefore, **this Guidance is complementary to what is already presented in those documents.**

With the European Green Deal (European Commission, 2019) the European Commission (EC) aims to transform the European Union's economy to support a more sustainable future and to implement the United Nations' agenda 2030. Among the objectives of the Green Deal is the Zero Pollution Ambition (European Commission, 2021b). To act toward this goal, a set of actions was outlined in the Chemicals Strategy for Sustainability (CSS) (European Commission, 2020). Specifically, within the CSS action 2.1 - Innovating for safe and sustainable EU chemicals, sub-action 2.1.1 aims at promoting safe and sustainable by design chemicals, while the sub-action 2.1.2 aims at achieving safe products and non-toxic material cycles. In 2022, the EC adopted a Recommendation establishing a European assessment framework for 'safe and sustainable by design' chemicals and materials (hereafter SSbD) in R&I activities to support the implementation of the CSS (European Commission, 2020). The scientific-technical basis, i.e., the SSbD framework, which the Recommendation is based upon, was developed by the Joint Research Centre (JRC) (Caldeira. et al., 2022a).

The SSbD framework aims to support decision making during the innovation process towards safer and more sustainable chemicals and materials over their life cycles. As such, the SSbD framework provides a set of assessments and indications aiming at this goal. The SSbD framework is flexible and can be adapted to specific organisation needs, structures and ambitions to stimulate safe and sustainable innovation.

The published SSbD framework was applied to case studies on selected chemicals, which increased the knowledge on the applicability of the framework and insights into relevant refinements. The report on the application of the SSbD framework to case studies (Caldeira et al., 2023) lists some of the challenges identified both via the case studies and as described by practitioners at the Stakeholder Workshops. Feedback on the framework was collected via a dedicated survey. Until the end of 2024, stakeholders have the opportunity to test the SSbD framework and to provide further feedback, suggestions, and report on challenges regarding its implementation.

The active **involvement of stakeholders throughout in the development and testing of the framework is crucial** to ensure and improve the applicability and workability of the SSbD framework in different value chains**.** The SSbD Framework will be revised, reassessed

and is expected to be reissued in 2025 in its second and revised version, after considering feedback received from stakeholders and users during the two testing phases and discussions at the several workshops and ad hoc submissions.

2 The SSbD framework in a nutshell

What is the SSbD Framework, and is it mandatory? What is the goal of SSbD?

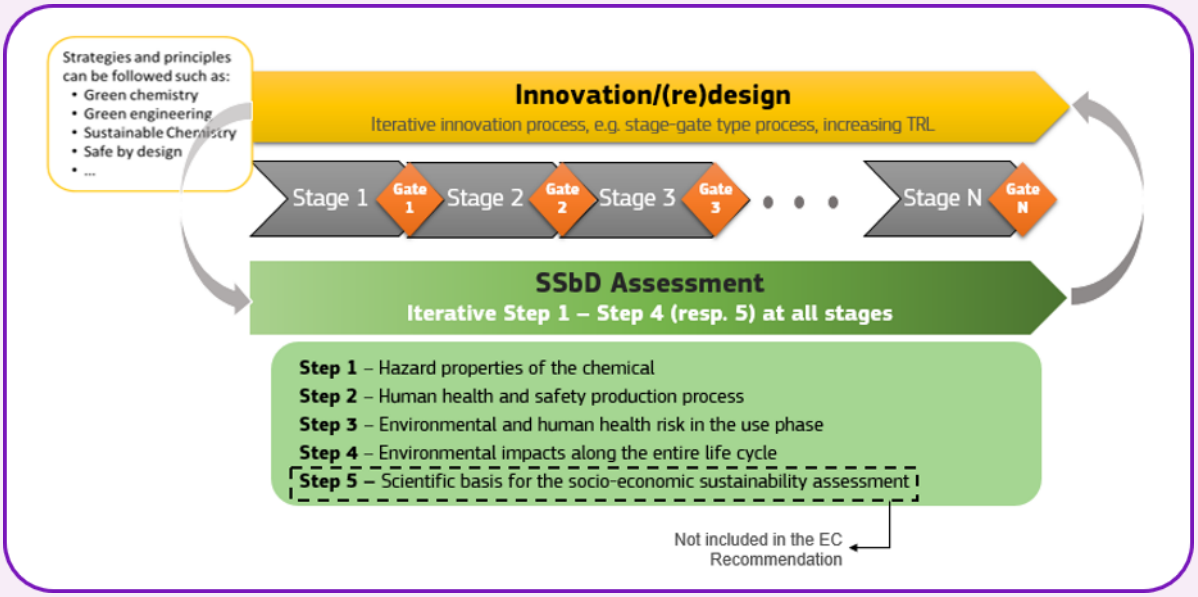
- The SSbD Framework is a general approach to steer innovation towards safe and sustainable chemicals and materials throughout the entire life cycle. The framework can be applied to the development of new chemicals and materials or to the re-assessment of those already in existence.
- The application of the SSbD Framework is **voluntary**. It combines established hazard and risk assessment approaches for chemicals and materials, with sustainability assessment techniques, such as Life Cycle Assessment (LCA) methods.
- The SSbD Framework has been developed as a specific action of the CSS, to promote the design, development, production and use of completely new safer and more sustainable chemicals and materials considering their entire life cycle, steering the substitution of hazardous and less sustainable chemicals and materials. The overall goal is to help in preventing pollution whilst also reducing society's environmental footprint.

What does the SSbD Framework consist of?

Figure 1 shows the two components of the SSbD framework:

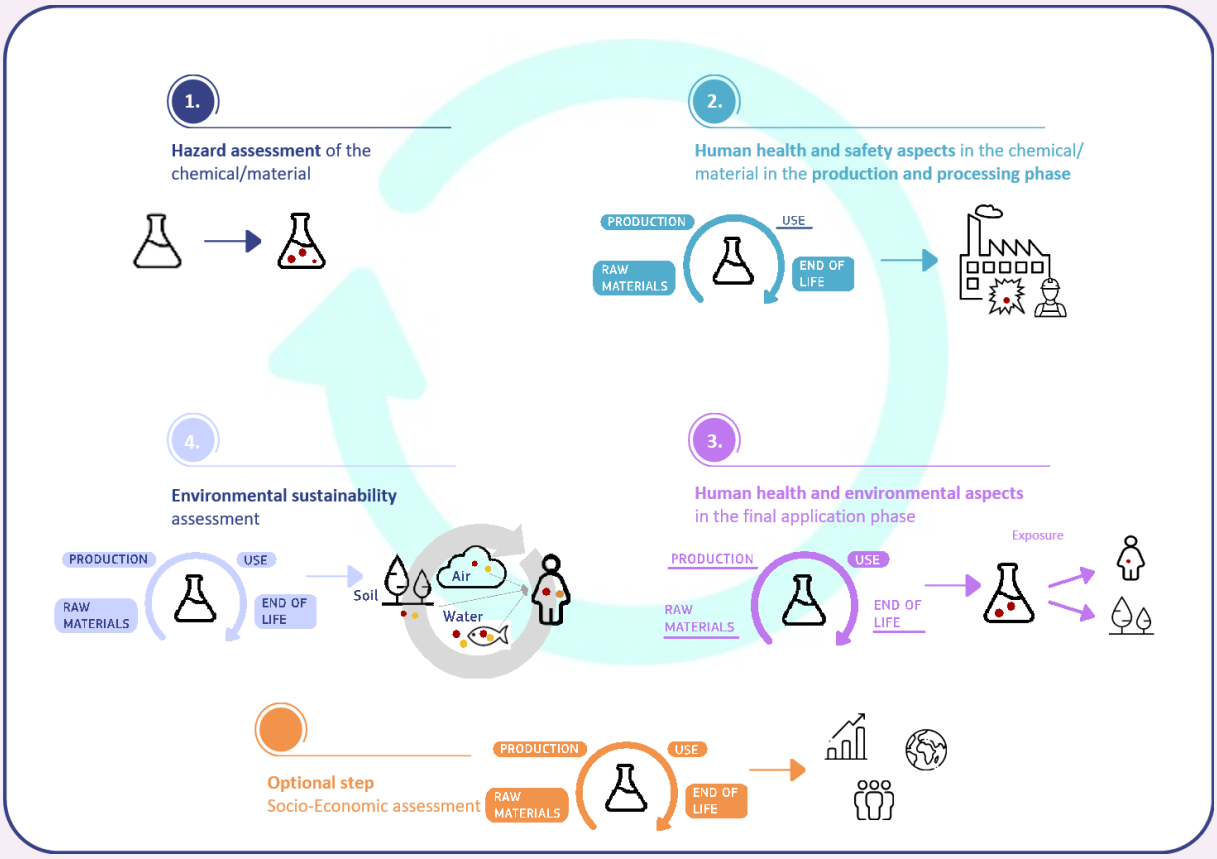
- A **(re)design phase**, based on general SSbD design strategies and principles, which come from existing concepts, such as Green Chemistry, Green Engineering, Sustainable Chemistry and Circularity. Examples for such strategies and principles can be found in Figure 5.
- A **4-step assessment phase**, with an optional socio-economic step.

Figure 1. Overview of the SSbD framework



Source: Own elaboration

Figure 2. Steps of the SSbD framework



Source: Own elaboration

The SSbD Framework

- is **voluntary**, and as such organisations are free to complement in-house design principles with those from the SSbD for **the innovation/(re)design phase;**
- is **iterative.** The assessment iterations take into account the gradually increasing amount of data generated and collected as the innovation proceeds. Risk and environmental assessments are performed at each iteration to the level of detail that can be achieved with the data available at that point in time;
- requires the innovation process to be **evaluated periodically**, e.g. via a stage-gate type approach, with regard to its overall goals (e.g. producing a less hazardous chemical for a specific application) whilst in parallel applying the SSbD framework. From the combined results obtained, the innovator determines whether the process will be continued.

How and when should the SSbD Framework be applied? What if there is only incomplete information on the sustainability aspects/safety elements?

- It is recommended to start applying the Framework as early as possible in the innovation process.
- As the application of the Framework is iterative, it can begin with the use of available information, using simplified estimation tools and models with narrower system boundaries, gradually building up and refining the information base over time. A lack of in-depth knowledge regarding safety and sustainability information is normal in the early innovation process. As the process is progressively refined, the innovation matures in parallel together with the completion of information gaps.
- The SSbD Methodological Guidance outlines the way in which the user can set the goals and scope and use established

and novel assessment means from an early point on, for Safety Assessment and Sustainability/Life Cycle Assessment (LCA).

How does the SSbD Framework link to existing assessment methods and tools?

Innovators that already have established R&D, safety assessment and life cycle assessment programmes can apply the SSbD framework. However, it is not necessary to have such programmes in place – the Methodological Guidance is written for everyone and helps identify available methods and tools.

How does the SSbD Framework promote innovation?

The SSbD Framework promotes the use of new scientific and technological knowledge and links together established assessment methods and tools:

- To avoid "reinventing the wheel";
- To use appropriate available data, as well as chemical risk assessment and life cycle assessment tools;
- That apply 'green' design principles, which mutually aid and reinforce the (re)design of safe and sustainable chemicals and materials;
  To feed into the overall process of corporate and R&D decision-making, including assessing trade-offs between various aspects: sustainability, safety, as well as socio-economic assessment along the whole life cycle.

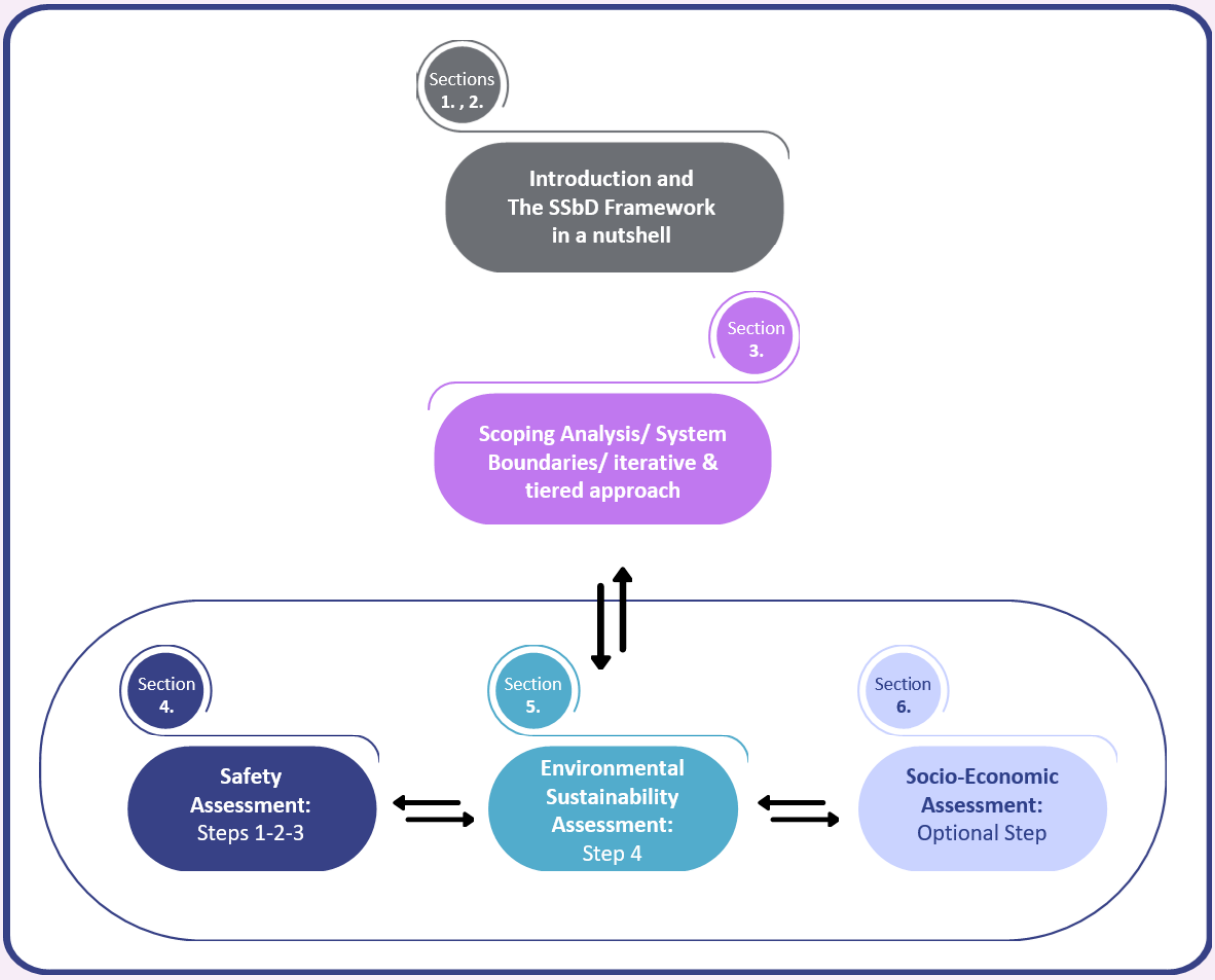
What are the links between the SSbD and established or upcoming regulatory requirements on safety and sustainability?

- The application of the SSbD framework is strictly voluntary and is oriented towards organisations wishing to consider general corporate responsibility in their innovation processes. Organisations can use the SSbD framework for their own Environmental, Health and Safety Management Systems, in-house auditing and review processes.
- The voluntary nature implies that there are no guarantees that the use of the SSbD framework (principles) automatically results in complying with particular regulatory requirements.
- Nevertheless, the use of the SSbD framework can be a tool that helps to meet regulatory needs, e.g. in the search for alternatives for substances that, today, can only be used under time-limited authorisations or exemptions from restrictions.
- Moreover, the SSbD framework can be used as an element in strategically developing a company's readiness with regard to future legislation that may require the use of "safer and more sustainable chemicals, processes and materials" to replace substances of concern.

What are the different parts of the Methodological Guidance of May 2024 supporting the implementation of the SSbD Framework?

The structure of the SSbD Methodological Guidance is shown in Figure 3.

Figure 3. Structure of the Methodological Guidance



Source: Own elaboration

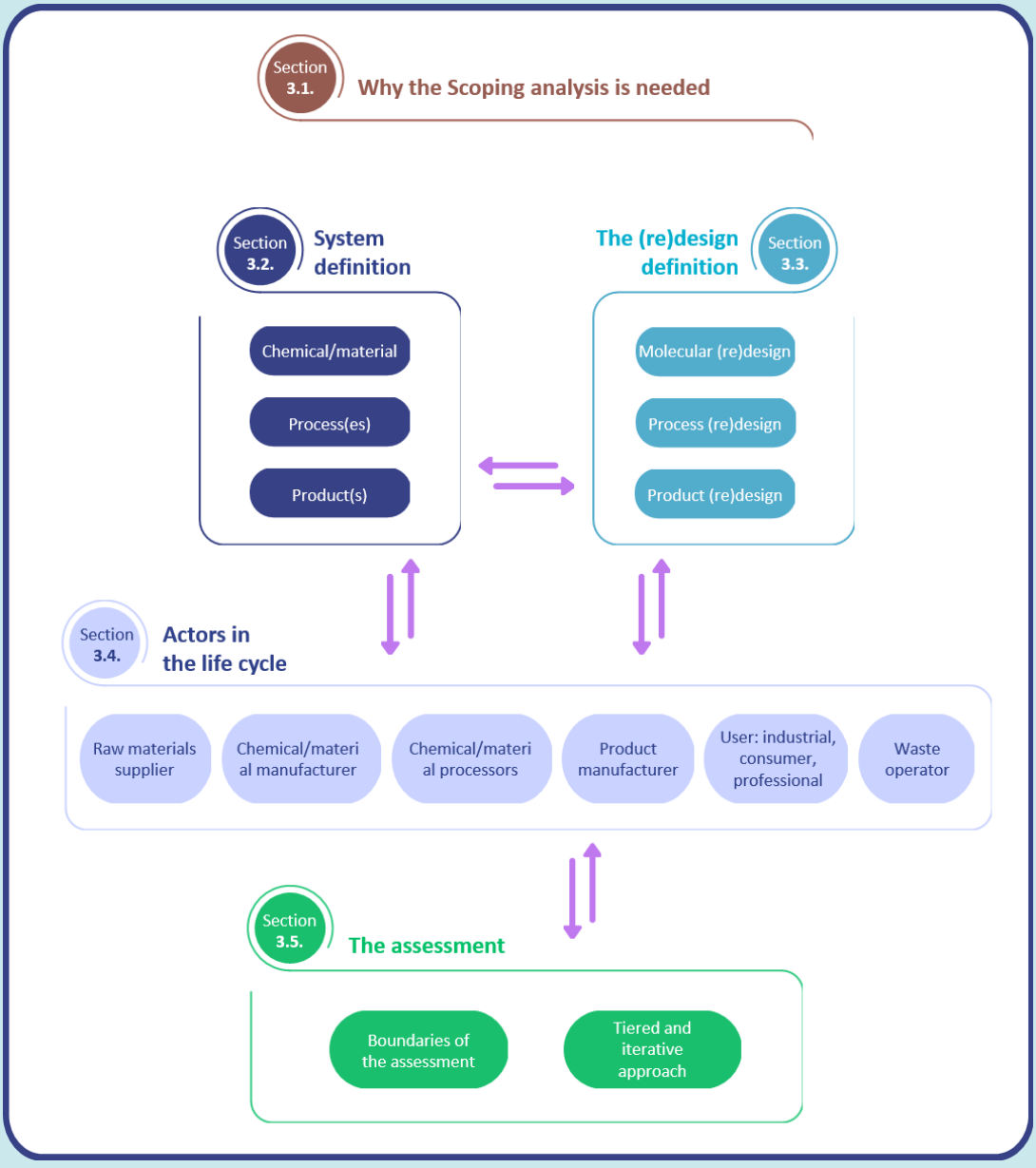
3 Scoping analysis and SSbD assessment

AIM OF THE SECTION:

The Scoping Analysis helps the implementation of the SSbD framework according to (re)design aspects, and maturity of the innovation itself. This section describes:

- The **information** needed to define the SSbD system to be assessed, such as:
    - The engagement with the SSbD system partners for the application of the framework
    - The nature and purpose/objective of the (re)design of the SSbD system
- The **iterative** and **tiered** SSbD assessment

STRUCTURE OF THE SECTION:



Source: Own elaboration

3.1 Why the scoping analysis is needed

The starting point of any kind of assessment is the scoping of its purpose, which is the process of identifying and prioritising the key issues associated with a project which need to be assessed. Scoping determines the boundaries and provides focus for the SSbD assessment in the broader R&I process.

An R&I project can be initiated from different needs, have different objectives, and involve different organisations.

For example, the innovation can be initiated by:

- An RTO (Research and Technology Organisation) providing innovative solutions to an existing product (e.g. a plastic container) to improve its performance in the application (e.g. improves the shelf life of the food in the plastic container)
- Consortia developing a tool to predict safe and sustainability performance
- A company exploring new bio based raw materials
- A company implementing a new production process
- A product manufacturer improving the safety, sustainability, and effectiveness of the product by changing how it is applied
- A manufacturer developing a new chemical/material

The application of the SSbD framework can be the common denominator guiding and supporting the innovation process with the objective of ensuring the safety and sustainability of the entire life cycle of the chemicals/materials addressed in such R&I projects, while also considering functional performance of the chemical/material. Application of the SSbD framework should ensure that any improvements made during the innovation have led to an improvement in one or more safety and sustainability dimensions without detriment to the others.

The scoping analysis builds on: the system definition, the (re)design definition, and engagement with the actors along the life cycle. The three building blocks are necessary, but can be implemented in a different order based on cases. At the end of the scoping analysis, the safety and sustainability assessments will be performed in an iterative and tiered way.

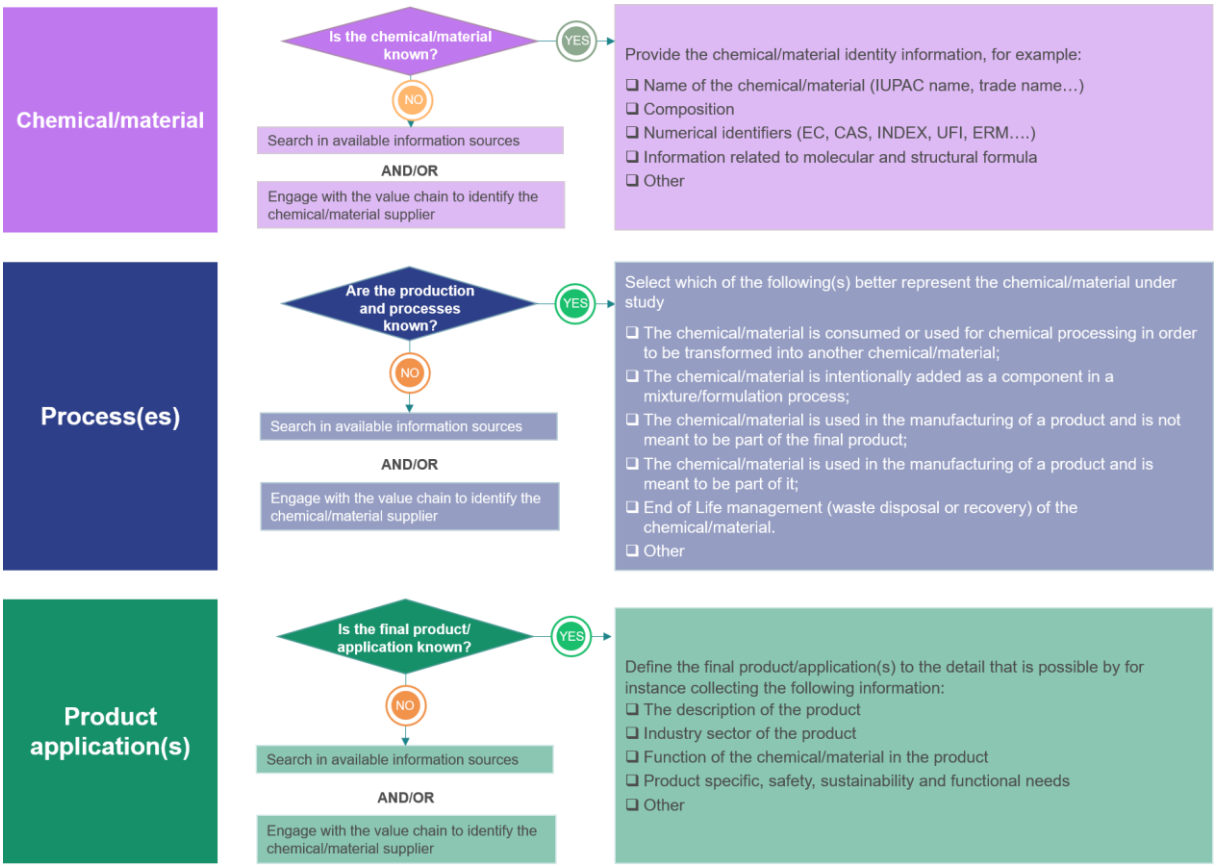
The scoping analysis aims to define the system under study for safety and sustainability assessment. The sections *Problem formulation* (Section 4.1) and *Goal and scope definition* (Section 5.2) help to further specify the study for the safety and environmental sustainability assessments, respectively.

3.2 Definition of the system under study

The definition of the system under study can be performed following Figure 4 (in addition, Table B.1 in Annex B). It includes: the chemical/material under assessment (chemical/material), its function (final product/application) and the considerations of the life cycle, including relevant processes and products (value chain). The starting point of the definition of the system to be assessed will depend on the organisation's position in the life cycle of the chemical/material. The system should always cover the three elements (chemical/material, process(es) and product) that are needed to define the boundaries for the assessment (see Section 3.5.1). Table 1 provides additional information regarding the importance of defining the system under study.

At the end of the identification process, the assessor should be able to define the entire SSbD system with all the different life cycle stages that need to be considered for the SSbD assessment (Section 3.5.1).

Figure 4. SSbD system elements (chemical/material, process and product) and information to define them



Source: Own elaboration

Table 1. Scoping analysis. Definition of the system under study

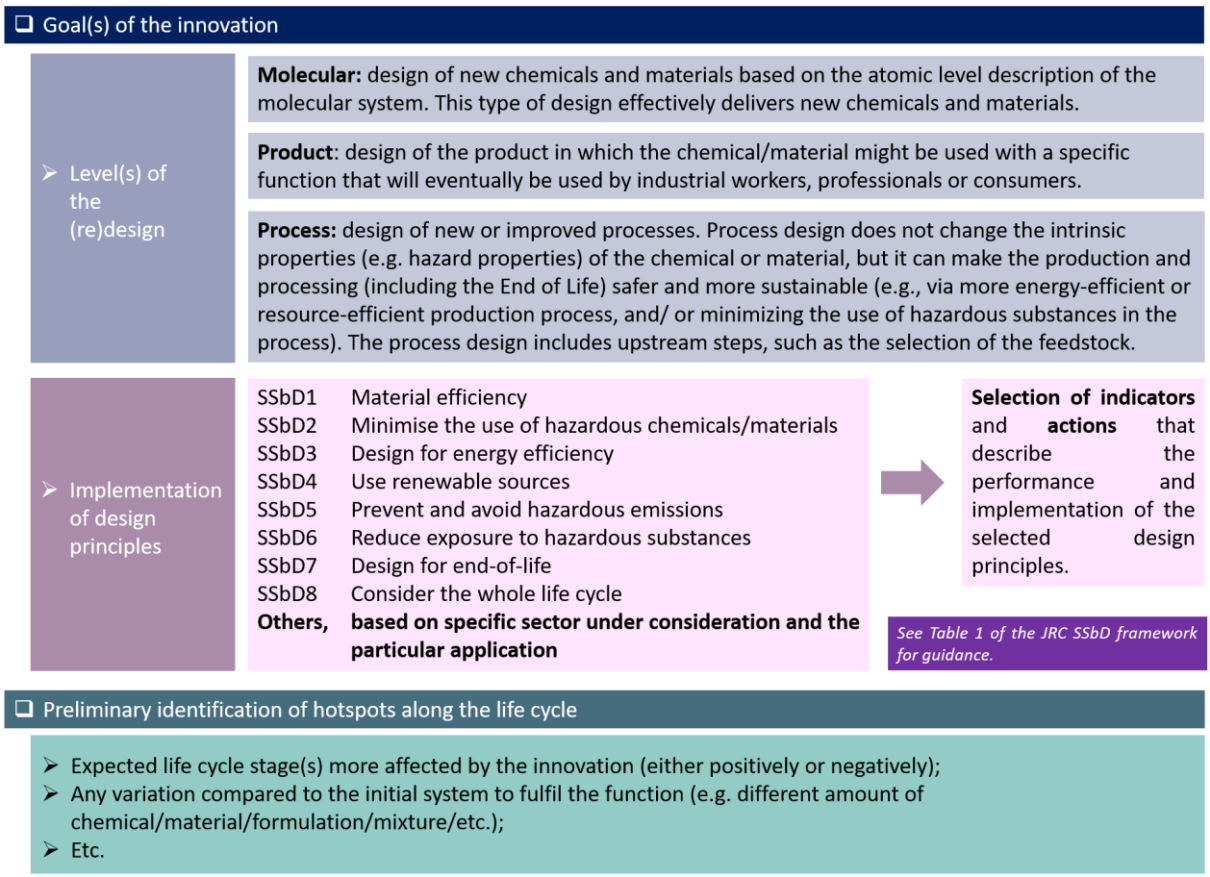
Identification of	Why it is needed	What the innovator should consider
Chemical/material	The identification and definition of the chemical/material is key as its intrinsic properties are determinant for both safety and sustainability assessment. The identification of the chemical/material will also support the identification of the processes and products of which it is a part and in which its intrinsic properties will have an impact.	REACH (European Parliament and the Council, 2006) and CLP (European Parliament and the Council, 2008), the fundamental EU chemicals legislation, do not define the term 'chemical', but rather define and distinguish the legal terms 'substance' and 'mixture' in the context of chemicals: **Substance:** A chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition. (EU, 2006) **Mixture:** 'a mixture or solution composed of two or more substances' (European Parliament and Council, 2006 as amended by EU, 2008) With regard to the definition of 'material', the SSbD framework defines: **Material**: substances or mixtures which may or may not fulfil the definition of an article under REACH and may be of natural or synthetic origin (European Commission Directorate-General for Research and Innovation, 2021). The SSbD covers both chemicals and materials and therefore the parameters for the identification can differ from case to case.
Process(es)	A very important aspect for the safety and sustainability assessment is how the chemical/material is manufactured and further processed. This is of paramount importance, because while the intrinsic properties of the chemical/material remain unchanged during the entire life cycle, the impact of the chemical/material will be specific to how it is used. Identifying the processes, the assessor will be able to assess the chemical/material impact to the target population in these activities.	The definition of the process starts with the identification of the activities of the first actor in the life cycle of a chemical/material, the manufacturer/producer of the chemical/material, and includes processes by which the chemical/material is produced from raw materials. It continues with the description of the processing activities like formulation where relevant, and/or other activities undertaken by workers. Products containing the chemical/material can be used or further processed by workers at industrial sites. This also includes processing of semi-finished products with the aim of producing the final product (e.g. calendering, spraying, extrusion). Activities related to the End of Life (waste disposal or recovery) are also considered.
Product/application(s)	The identification of the final product/application enables the assessor to explore how the chemical/material is used, and also assist the understanding of the role/impact of the chemical/material in the safety, sustainability and functionality performance in the end product and application, notably in the population exposed to it. Identifying the processes, the assessor will be able to assess the chemical/material impact to the target population in the final product/application.	As much detail as possible regarding the product/application is relevant for scoping the SSbD assessment. The identification of the industry sector and type of product are often identified at the beginning of innovation. The assessor should consider the particular function (or service) that the chemical/material provides to the product/application. Another important aspect is the identification of regulatory requirements related to safety and functionality performance that the product/application must fulfil for the innovation to be placed on the market.

Source: Own elaboration

3.3 Definition/identification of the (re)design

The definition of the SSbD system is completed by defining the (re)design aspects. These aspects require the description of the goal(s) of innovation, and the preliminary identification of potential hotspots along the life cycle. Figure 5 provides a guidance on the useful information to collect to define the (re)design. Additional information might complement the definition of the (re)design.

Figure 5. Information to collect for the (re)design definition



Source: Own elaboration

The **goal(s) of innovation** trigger a series of questions, for example: What are the principles on which the (re)design is going to be based? What are the needs to improve/ensure the safety, sustainability, and functionality within the SSbD system? Which elements of these considerations will be addressed and assessed, and in what degree of detail?

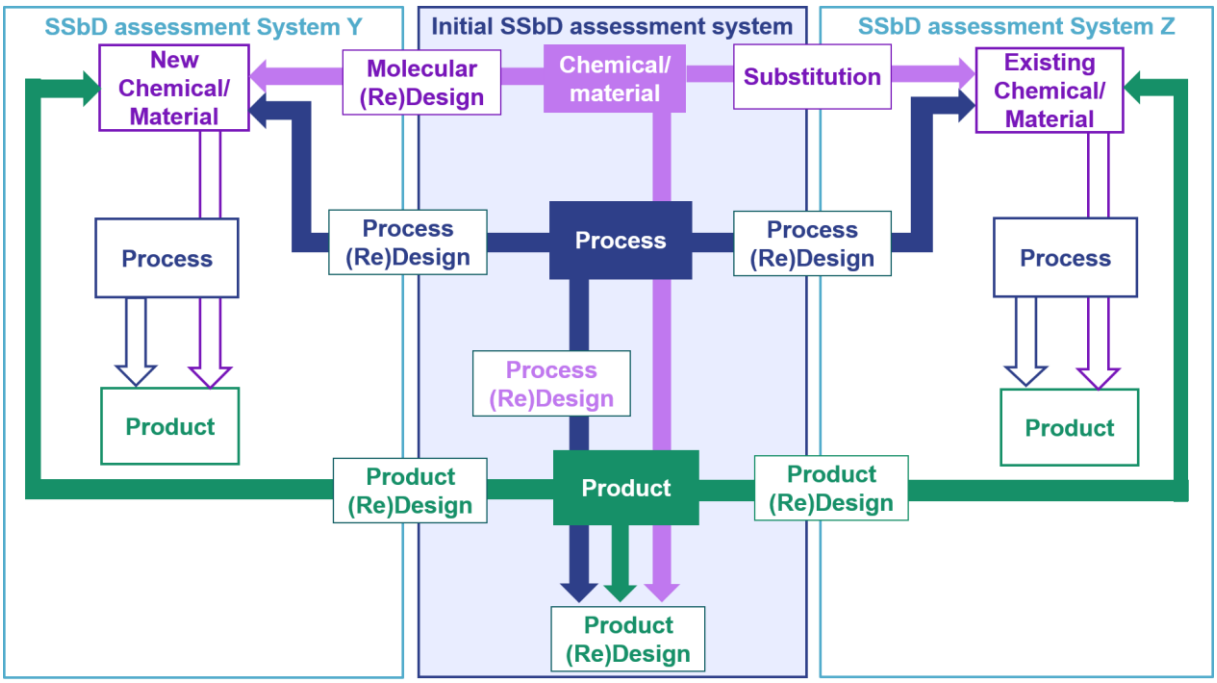
Hence, the first type of information to collect might be the **level(s) of the (re)design, following** the definition given by the EC Recommendation (European Commission, 2022a).

The second type of information refers to the use of design principles (as shown in Figure 6), with the accompanied indicators and actions. **The list of the eight SSbD design principles is illustrative and not exhaustive; it can be expanded according to the needs of the specific sector under consideration and the particular application**. The indicators can be used as a starting point to perform the assessment based on their direct link to specific principles. Box 1 presents an example of an innovation with the goal of improving circularity (End of life) of a product and associated considerations for the implementation of the SSbD framework.

The **identification of preliminary hotspots along the life cycle** helps to frame the assessment on potential consequences due to the innovation. The innovation might trigger questions such as if there is any variation compared to the initial system to fulfil the function (e.g. different amount of chemical/material/formulation/mixture) or if the innovation might involve the use of a chemical/material not used in the initial system under study. This variation in the initial system is shown in Figure 6. The chosen (re)design might lead to the need to assess a different (new) SSbD system. This is because the chosen (re)design might introduce differences in e.g. the chemicals/materials used, the process or the product design, which will define a new system to which the framework should be applied.

As the innovation evolves, the need to change to yet another SSbD system may arise, which leads to the situation that within one R&I project, the SSbD framework needs to be applied to more than one relevant system, e.g. the initial system and systems Y and Z in Figure 6. The example shows that, depending on the type of innovation (e.g. substitution of a chemical/material with an already existing chemical or designing/developing a new chemical) the systems to be assessed are different. It is thus important to identify the different SSbD systems from the beginning, or as early as possible. Box 1 provides an example of the links between the initial SSbD system with other SSbD systems.

Figure 6. Changes in the initial SSbD system, depending on the nature of the (re)design, the initially defined SSbD system might change during R&I projects



Source: Own elaboration

Box 1. Link between the (re)design and the implementation of the SSbD framework

Example 1: Paint producer

Different (re)design aims can be envisaged, and two of these would be:

(a) Reducing the inhalation exposure to the consumer/professional user during application. The paint could be applied with a brush instead of being sprayed. There would be a need to assess whether this will affect other aspects and dimensions of the SSbD such as environmental releases, End of Life, or waste. Nevertheless, as the system always depends on the chemical/material, in this case the SSbD system assessed **remains the same**.

(b) Substituting a SVHC (Substance of Very High Concern) in the paint. The SSbD system **changes** as the chemical/material under assessment changes and the new system needs to be assessed in order to evaluate its safety and sustainability performance in addition to its technical functionality through the entire life cycle and considering all the SSbD steps.

Example 2: Design for end-of-life for critical raw materials (CRMs)

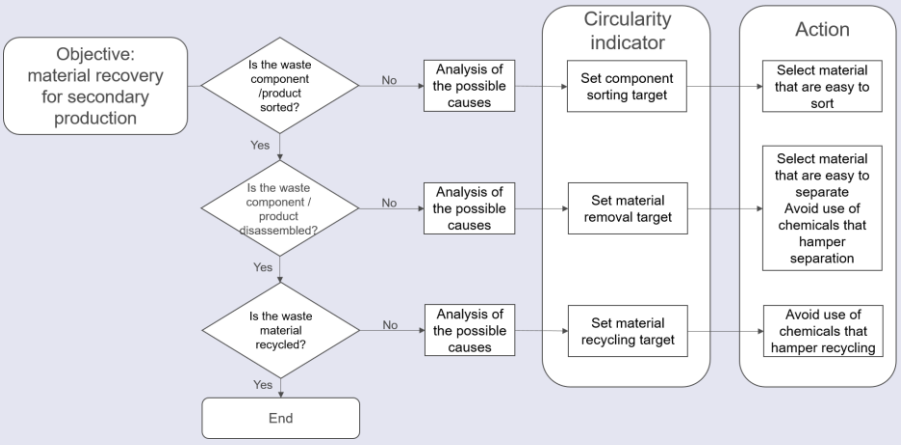
The possibility of recycling and disassembling are crucial indicators to ensure the recovery of CRMs, thus avoiding the potential negative environmental and social impacts associated with their extraction and processing, and Step 4 and the socio-economic assessment would have a particularly relevant role in the assessment.

Figure 7 shows a general example of how the 'Design principles' could be considered to capture the circularity aspect of a material embedded in a component or product and to identify the 'hotspots' of the waste management operations, to place the most effective corrective actions.

At the beginning, the specificities of the waste component/product and the related waste chain should be analysed to identify the real 'gaps' to achieving circularity of the material and related causes (e.g. infrastructural deficiencies, presence of chemicals that hinder the waste management operations). Thus, the adoption of the most suitable indicators and of the set targets, via the adoption of the proper actions, could guide the company towards the (re)design phase. Any actions and target set hence need to be analysed in the subsequent part of the implementation of the framework by the SSbD assessment.

The outcome of the decision flow could affect the entire 'SSbD system' (see Section 3.2), since it addresses the 'Chemical/material definition'.

Figure 7. General flow for implementing the 'Design principles' within the (re)design phase, which is in this example the 'Design for end of life'



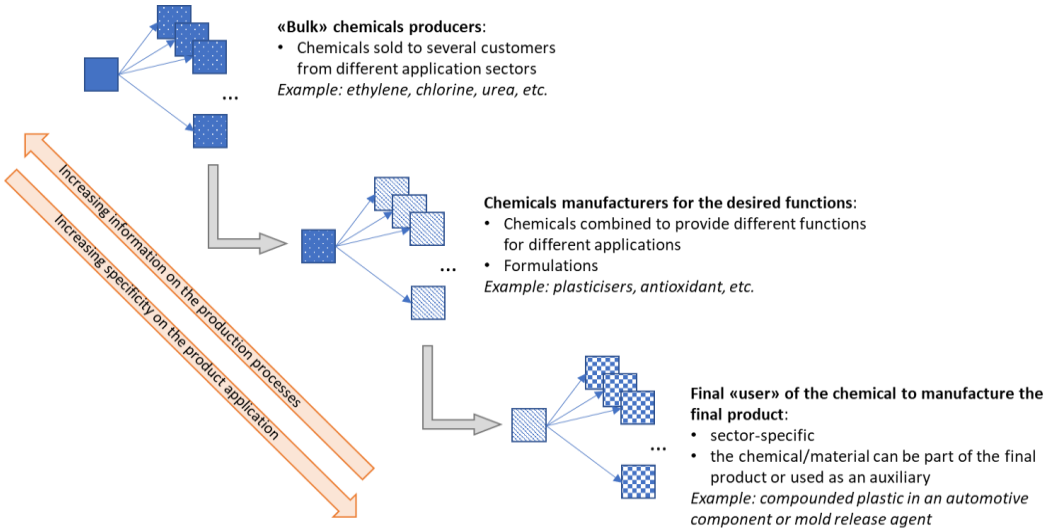
Source: Own elaboration

3.4 Identification and engagement with actors of the life cycle

The inclusion of the life cycle perspective highlights the importance of the value chain, making it clear that the application of the SSbD framework goes beyond the responsibility of a single stakeholder and instead envisages the involvement and collaboration of all stakeholders along the value chain. Hence, all the actors involved in the life cycle of a chemical/material have a role and a responsibility in ensuring that the chemical/material, process, and product is safe, sustainable, and functional (Figure 8).

It is recognised that the identification of all involved stakeholders is one of the biggest challenges in the implementation of the SSbD framework, and in the SSbD assessment it is thus **important to identify the actors involved in the life cycle** of the chemical/material assessed, starting from the raw materials and until end of life. The scoping of the SSbD assessment and definition of the SSbD system will clarify the position of one's organisation and will assist in identifying actors/stakeholders in the value chain and engaging with them early in the R&I process.

Figure 8. Conceptual example of a simplified supply chain of a chemical/material, including the number of actors involved and the possible data and information flows



Source: Own elaboration

Upstream in the value chain is the production associated with the chemical/material, and available information would be for example on the manufacturing process(es) of the chemical/material and their inherent properties. The chemical/material often passes through different processes and ends up being part of a plethora of products. However, information on these might only be partially available to the upstream manufacturer. On the other hand, downstream end users possess all the information related to their own processes and uses, but often are lacking information on the chemical/material properties.

Therefore, the identification of the actors/stakeholders in the value chain will also help to identify the roles and responsibilities in the context of safety, sustainability, and functionality performance in the value chain. Furthermore, a shared effort in meeting the ultimate goal of SSbD would represent a strong advantage regarding possible future requirements (for safety and/ or sustainability) when placing the chemical/material on the market.

The information exchange will, at least in part, rely on the creation of a trusted environment for communication and collaboration among actors in the value chain (See Figure 9).

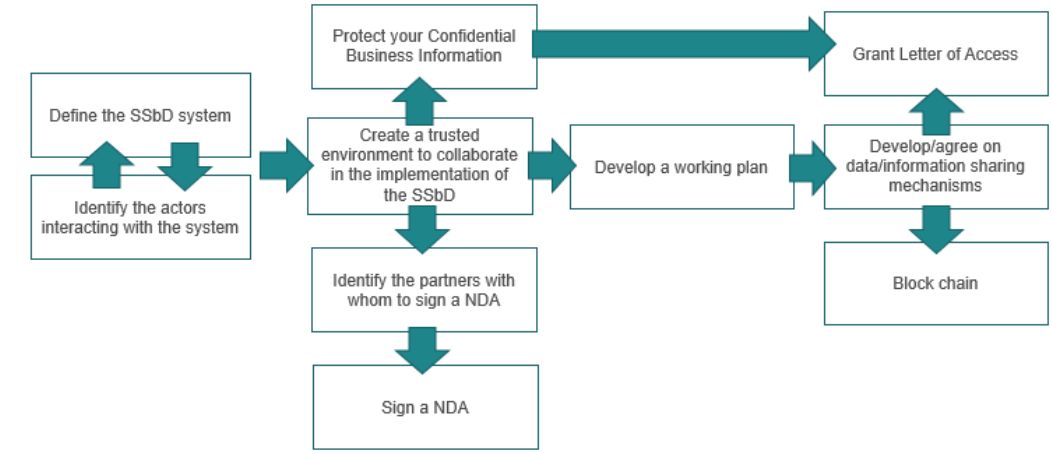
One of the instruments used for these purposes are Non-Disclosure Agreements (NDAs) (GOV.UK, 2024). A NDA is a legally binding contract that establishes a confidential relationship between two or more parties. It can be either unilateral, when one party that holds sensitive information, and the other party that will receive that sensitive information; bilateral, when both parties hold and receive sensitive information; or multilateral. Depending on the length, complexity and additional factors, stakeholders can decide which NDA better suits the specific case.

Other points that might need consideration are business confidentiality and intellectual property rights related to the data. Some of the data or information needed for the assessment of the safety, sustainability, or functionality performance might be considered by stakeholders in the value chain as Confidential Business Information (CBI), which is a valuable asset that needs to be protected.

Should the use of CBI data be needed by other actors in the value chain, the most common practice is to grant access to this protected data in the format of a "licence to use", granting legitimate possession of the data or "letter of access", granting the right to refer to the data for specific purposes e.g. SSbD.

Another important aspect to take into consideration is how this data and information can be shared in a way that it is findable, accessible, interoperable, and reproducible by all value chain actors and sharing it in a secure and encrypted way such as Block Chain. Figure 9 show a possible connection of the actions described.

Figure 9. Actions to be considered during the SSbD implementation to identify and create a trusted environment among value chain actors



Source: Own elaboration

The implementation of the SSbD framework will be limited in case the assessor has only little interaction with the actors in the value chain. In such situations, the implementation would be based only on data available to the assessor and would necessitate more assumptions.

3.5 SSbD assessment

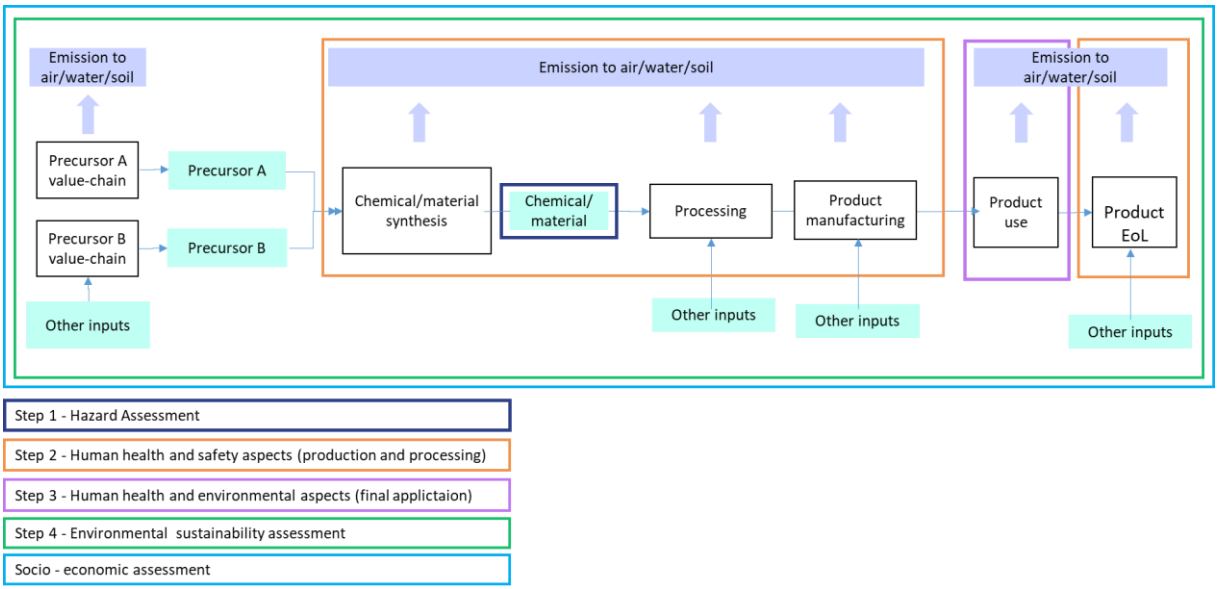
3.5.1 Definition of the boundaries of the assessment

The next step in the scoping analysis builds on the defined SSbD system to identify the entire value chain and to set the system boundaries for the safety and sustainability assessment.

These boundaries will describe what should be considered in the assessment and what should be left out. Defining the system boundaries will also aid the assessor to identify which stage of the life cycle

falls into which step of the SSbD assessment and in which of them the (re)design might have a bigger impact, as illustrated in Figure 10. The colour-coded boxes in the figure link the SSbD assessment steps to the relevant stages in the life cycle.

Figure 10. Representation of the alignment between the chemical/material life cycle and the progressive required broadening of the SSbD assessment steps and boundaries (boxes in white are processes stages, coloured boxes are inputs and outputs of the processes). [EoL: end of life]



Source: Own elaboration

The definition of the boundaries and the identification of the information needs will be an iterative process that will need to be revisited at each iteration of the assessment. Also, each iteration will determine the type of assessment and the associated uncertainty that is acceptable in order to ensure its adequate performance.

3.5.2 Iterative and tiered approach for the SSbD assessment

The SSbD framework can be applied at any moment of the research and innovation process. The aim of the application of the SSbD framework in R&I processes is to support the design and development of safe and sustainable chemical and materials. Hence, it is ideal to implement the SSbD framework from the beginning and throughout the entire R&I process, in an iterative and tiered approach.

The **iterative approach** of the SSbD follows the iterative nature of any innovation. Hence, several iterations of the SSbD assessment are carried out along the innovation. The iterations of the SSbD assessment might be, for instance, linked to the increasing knowledge of the innovation, as well as to the data availability and quality for the assessment.

The **tiered approach** gradually completes the SSbD assessment with the increasing available information over the development of the chemical/material, processes and products, together with an increasing certainty regarding the results obtained in the safety and sustainability assessments.

Based on these two approaches, this section presents a general structure of the SSbD assessment that can be implemented along the R&I processes, following:

- The number of alternatives (i.e. process improvements, chemicals, materials, applications, etc.) under evaluation;

- The availability and uncertainty of the data;
- Other aspects that might affect the assessment and the innovation.

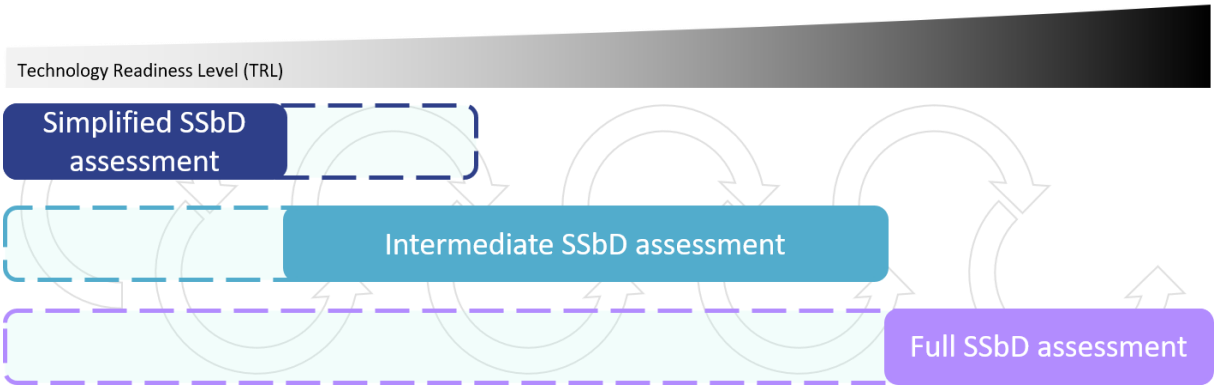
Figure 11 shows the overall structure of the tiered and iterative approach described by three main levels of the SSbD assessment, which go from a simpler to a more complete version, following the Technology Readiness Level (TRL) of the innovation (Buchner et al., 2019).

Table 2 describes the overall structure of each of them and the main aspects. For further guidance, please follow the indications in the table.

It has to be noted that the structure of the approach of the SSbD assessment:

- Is an attempt towards the integration of the tiered and iterative approaches both in safety and sustainability assessments; and
- Supports the implementation of the SSbD framework toward the completion of the SSbD assessment.

Figure 11. Overall structure of the iterative (arrows in background) and tiered (increasing maturity of the innovation) approach of the SSbD framework along the chemical/material innovation, following the TRL (Buchner et al., 2019)



Source: Own elaboration

Table 2. Description and applicability of the tiered approach of the SSbD assessment

	Simplified	Intermediate	Full
Description	It captures uncertain and unknown information regarding the chemical/material-related innovation. It is mostly guided by the goal of innovation, and identification of hot-spots. It can include screening assessment	Starting from the simplified version of the SSbD, it comprises a set of iterations following the increasing availability of data, the definition of the innovation, etc.	It reflects the complete and full version of the SSbD assessment, as presented in the SSbD framework. This considers all the dimension, indicators, and aspects that guarantee a holistic assessment of the innovation
Applicability	For instance, when: - Several options are considered in the innovation - The TRL is quite low - Scarce knowledge of the innovation exists - Few data are available - Other limitations related to the innovation	For instance, when: - The simplified SSbD assessment has been completed - Reduced numbers of options considered in the innovation - The TRL is increasing - Increasing knowledge of the innovation is available - Increasing levels of data availability and quality exist	For instance, when: - Very few options are considered in the innovation - The TRL is quite high - Complete knowledge of the innovation is available - Good level of data availability and quality exist
Main methodological aspects Safety assessment (Step 1 to Step 3)	Some simplifications in the assessment can be made focussing on aspects that might raise concern in the Risk Assessment and will help filtering the innovation option, such as: - Physico-chemical and fate properties that might raise exposure concerns. - Hazard profile potential due to similar structures and structural alerts. - Relevant hazard properties for the identified uses. Existing databases and easy to use prediction tools can support the identification of red flags warning the innovation about: - The need for additional data - The need of higher tier assessment - The non-compliance with SSbD	The scope is expanded to cover all the aspects in a tiered Risk Assessment approach and as data becomes available. (See section 4) Engagement with the actors along the life cycle is important to fully picture the chemical/material life cycle, to identify all “uses” and collect further data for the refinement of the assessment (See Section 5.3). Both hazard (See Section 4.2.) and exposure (See section 4.3.) assessment contribute in an iterative and tiered approach to the overall Risk Assessment (See Section 0.) Generic information on chemicals/materials and uses can be retrieved from existing communication tools such as the extended Safety Data Sheets (See Section 4.3.2.1.) Prediction tools in combination with non-animal tests can support further progress in the generation of data. (See Section 4.2.1)	Full Risk Assessment considering the entire life cycle.

	Simplified	Intermediate	Full
Environmental Sustainability Assessment (Step 4)	Some simplifications to enhance the identification of hotspots: Narrowed system under study, representing the stages of the life cycle that are directly affected by the goal of innovation (go to Figure 10 of Section 3.5.1). See Section 5.2.3 for the Step 4. Simplified tools for data generation, or process simulation can aid the data gaps and the preliminary identification of hotspots (PARC Toolbox provides some existing options). Scenarios regarding exposure if the application is unknown, would be possible.	System boundaries: from cradle-to-gate to cradle-to-grave (See Section 5.2.3 for the Step 4) The number of iterations mostly focuses on the refinement of the Life Cycle Inventory. This requires - Efforts in the data collection: Primary data should be prioritised to secondary data (see Section 5.3 for additional information). - Engagement with the actors along the life cycle has to be prioritised to improve the modelling (See section 0). The full set of impact categories should be considered to obtain a holistic assessment of the chemical/material innovation.	Step 4 is recommended to be performed following the PEF/ Environmental Footprint method.
Example: Goal of the innovation: Substitution of Substance X with a less hazardous substance (molecular (re)design)	**Scenarios**: Substance X is used in several applications. Preliminary scenarios definition already in the scoping analysis with additional information for the safety and environmental sustainability assessment **Alternatives** might be several, but at the beginning of innovation based on the desired functionality for the described use/scenario. Possible **structure of the initial assessment**: Screening of the alternatives, focusing on relevant safety and sustainability aspects like specific intrinsic properties and narrowed impact categories (for Step 4). **Potential outcomes**: hotspots to consider when progressing in the innovation and critical aspects where more data needs to be collected or generated.	**Alternatives.** As the outcome of the simplified assessment several alternatives have been selected (new ones can be included along the innovation) to continue the innovation process. Possible **structure of the assessment:** Based on the outcomes of the simplified assessment, more data will be available, and refinement of the different assessment steps will be possible. **Potential outcomes**: This intermediate assessment will support the process of collecting and generating the appropriate information and the refinement and certainty of the assessment.	**Alternatives.** Possibly, alternatives A and B might reach this level of the innovation. Possible **structure of the assessment:** The number of the iterations of the intermediate level of the assessment will converge to the full SSbD assessment. For instance, refinement of the uncertainty, or Step 4 will be compliant with the EF method, and a holistic evaluation of the results coming from the steps is possible. **Potential outcomes**: Full SSbD assessment for the alternatives.

Source: Own elaboration

4 Safety assessment

AIM OF THE SECTION:

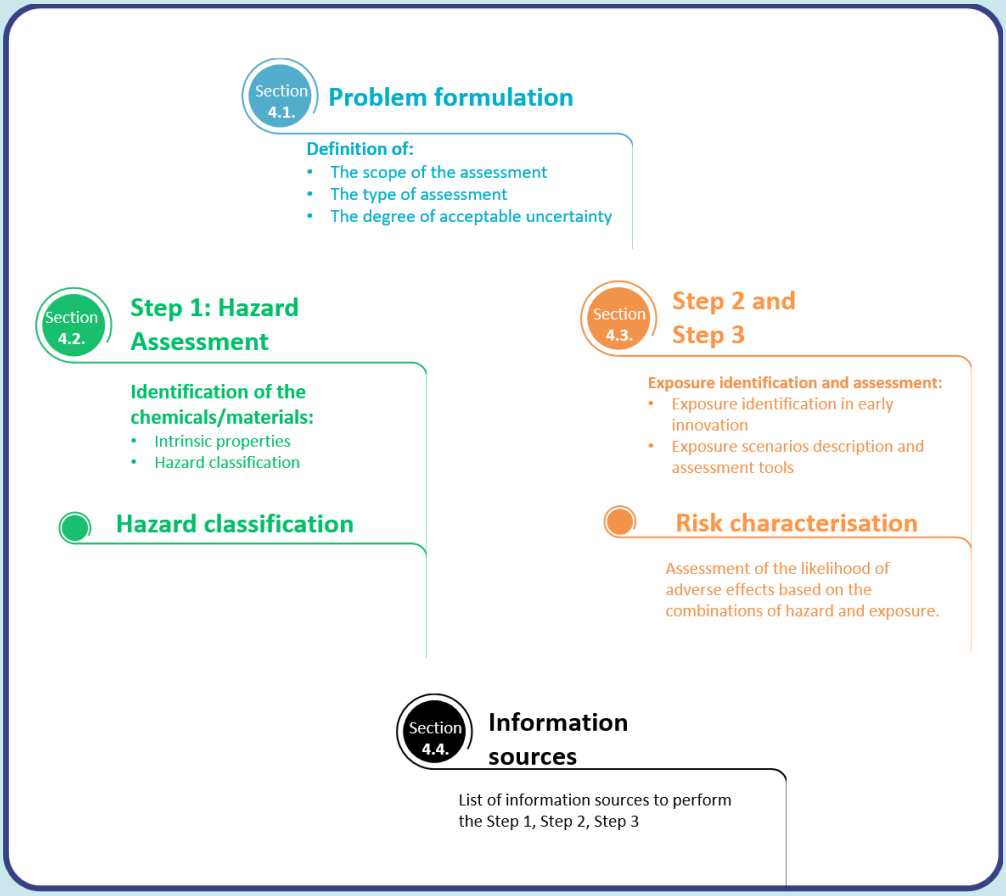
This section provides information to support the innovator in identifying the best approach for the risk assessment in an iterative and tiered manner as information becomes available and the quality and certainty increases. For guidance on how to perform a complete risk assessment e.g. ECHA's website should be consulted.

The section briefly covers:

- Step 1 Hazard assessment of the chemical/material.
    - Hazard identification: the approach for collection and generation of data for the hazard classification and
    - Hazard characterisation: the derivation of maximum exposure limits.
- Step 2 and 3: Safety aspects in the chemical/material production, processing, and final application.
    - Exposure identification and assessment
    - Risk characterisation

It also provides available sources of information for the purpose of developing the exposure scenarios.

STRUCTURE OF THE SECTION:



Source: Own elaboration

4.1 Problem formulation

The Problem formulation in the Safety assessment is complementary to the scoping analysis performed for the definition of the SSbD system, by considering additional information to perform Steps 1 to 3. For further guidance regarding the scoping analysis, please go to Section 3.

There are 2 different components that contribute equally to the safety assessment, and there are two main approaches for safety assessment based on these components:

- In the **hazard-based approach,** the nature of the hazard will determine the possible use(s) of a chemical/material while the hazard must be identified and characterised first. This approach can cause studies to be carried out unnecessarily, which uses unnecessary resources and tests.
- In the **risk-based approach**, the exposure combined with the hazard determines the risk. When the exposure is known, hazards can be assessed in a targeted way and targeted safety decisions can be made.

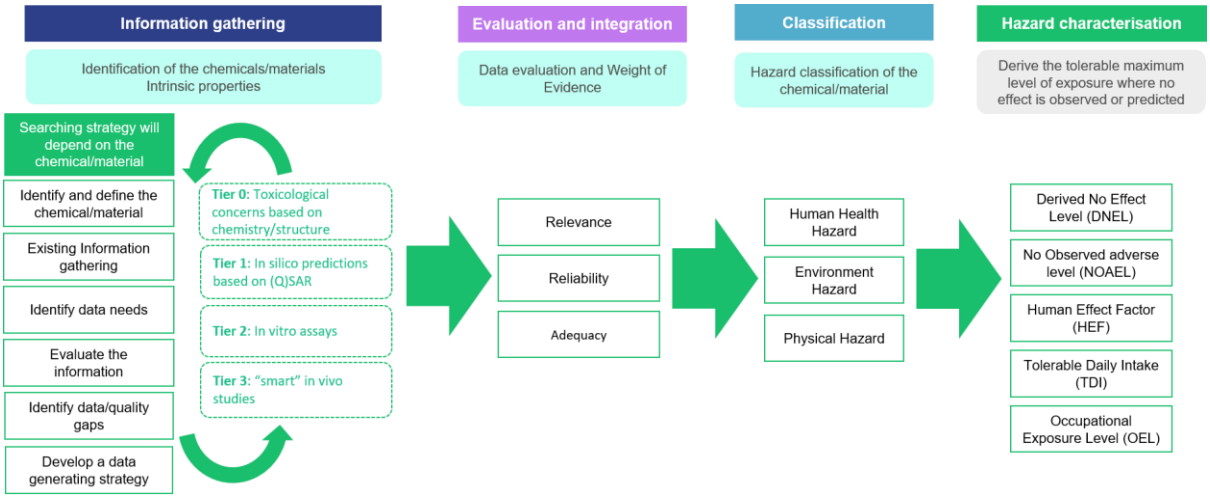
4.2 Step 1: Hazard Assessment

The relevant aspects for the hazard assessment are hazard identification and characterisation, as described in this section, they are shown in Figure 12.

The hazard assessment starts with gathering all relevant and available information. This is then followed by the hazard assessment per se of the available information, a process that comprises 3 elements which are part of the assessment in the following steps:

1. Evaluation and integration of the available data
2. Classification
3. Derivation of the hazard thresholds for the specific assessment target

Figure 12. Scheme of the relevant aspects for the hazard identification and characterisation



Source: Own elaboration

4.2.1 Data gathering and evaluation

The exact search strategy for a particular chemical/material will depend largely on its nature. Whatever strategy is employed, it is important to record which assumptions are made, what is performed and when it is done, as well as its outcome.

It should ideally consider the steps as follows:

- **i.** Identify and define the chemical(s)/material(s) under assessment (See Section 3.2)
- **ii.** Based on the problem formulation, the innovator should identify the data needs, e.g. quality (incl. uncertainty) and completeness, to give answer to the formulated problem.
- **iii.** Innovators should gather all available and relevant data with regards to the physicochemical, toxicological and ecotoxicological properties according to the identified needs.
- **iv.** Evaluate the reliability, relevance, and adequacy of the available information for arriving at conclusions in hazard assessment.
- **v.** Identify data and quality gaps according to the data needs and the problem formulation.
- **vi.** Develop a data generation strategy if needed to fill in the data gaps.

The process of gathering data is an iterative process that leads to a collection of more refined and higher quality data. The tiered approach associated with this iterative assessment may be looked at from different perspectives, and drawing conclusions in response to the problem formulation will depend on the success in problem formulation, adequately defining the data needs and the tolerable uncertainty levels. For instance, at the beginning of innovation, the assessor might prioritise the availability of data regardless of its quality and the associated degree of certainty to have an early indication of "red flags" (raising awareness of a potential hazard). Alternatively, s/he might prioritise instead the quality and certainty of data for a specific endpoint that raises a (potential) concern during the use of the chemical/material.

The collected and generated data in Step 1 give an overview of the toxicological properties of the chemical/material. From this information, the assessor should provide a response to the formulated problem of the hazard classification according to the Classification, Labelling and Packaging Regulation (CLP) criteria.

4.2.1.1 Information sources and tools for data collection and generation

A first hazard identification issue for chemicals/materials is the amount of data needed in relation to their intrinsic properties, in order to draw initial conclusions on their classification according to the CLP criteria. According to REACH, existing chemicals and materials must have certain data when placed on the market in quantities above one tonne per manufacturer/imported per year. However, for new chemicals and materials at low tonnages, the available data may be quite limited. Other legislation, e.g. the Biocidal Products Regulation, also have data requirements, but no tonnage triggers. Depending on relevance, the substance under scrutiny may already be classified based on that data. At the early stages of new molecular innovation, data is very scarce and new approach methodologies (NAMs) data, such as from *in vitro* tests, and *in silico* models and tools (e.g. quantitative structure–activity relationship models (QSARs)) are relevant means to support and guide the innovation process towards non-hazardous chemicals and materials, since they provide information that is relatively economical to obtain.

As in other methods used for data generation and evaluation, NAMs also have their limitations. NAMs need to be used and considered by experts, and utilised in conjunction with expert judgment, in order

to draw appropriate conclusions from the provided results. Another aspect which needs to be considered is that *in silico* tools usually build their prediction models based on pure chemical substances. Therefore, they may not be applicable to industrial substances or materials which can contain impurities or mixtures, which may not be well identified. The impact of impurities needs to be evaluated on a case by case basis. Mixture effects could, in principle, be assessed using principles of additivity, assuming that the mixture composition is well known, though the assessment must also recognise potential synergistic and antagonistic effects.

However, at the early innovation stages, there is a need to easily and reliably predict data to identify "red flags" as early as possible. As mixtures and materials are composed of substances, one way to identify these red flags is to choose the "substance/component approach". This way, specifically at early innovation stages the innovator/assessor may perform the assessment on individual components (substances) of a mixture or a material to address the data needs, using *in silico* tools.

The innovator should collect all available information, which can include:

- Information about the chemical/material identity
- Physicochemical data
- Non-testing data: i.e. data obtained with (Q)SAR models, grouping, read-across, weight of evidence etc.
- Testing data: including all in vitro and in vivo testing data, as available
- Human data, including epidemiological data, where available
- Any other data that may assist in identifying the presence or absence of hazardous properties

This information might be gathered from various sources:

- Internal sources available to assessor(s)/innovator(s)/trade association(s)/etc.
- Regulatory and scientific databases
- Scientific peer-reviewed literature and grey publications
- Internet searches
- Textbooks
- New Approach Methodologies (NAMs).

The search strategy will depend on the chemical/material specificities and the problem formulation (see above). Whichever strategy has been followed, it is important to record which assumptions have been made and why, what has been done following these assumptions and what has been the outcome.

The generation of new data should follow a tiered approach as information becomes available, and as the need for new data is identified by the problem formulation. Data generation should start with the most conservative expected toxicological concerns, based on the structure and chemistry of the chemical/material.

In a second tier, this information should be completed by looking for additional data and higher certainty levels with the use of *in silico* tools based on (Q)SARs. (Q)SARs can be an effective and efficient tool, especially for screening at early innovation stages, since they can identify "red flags" in a fast and economic way, and can help to correct the direction of the innovation before more resources are invested.

There is a plethora of models and tools integrating these models and a comprehensive overview is out of the scope of this report. In this guidance, the following examples of available QSAR resources are listed:

- The OECD **QSAR Toolbox** (OECD, 2024) is a type of software for retrieving chemical and toxicological data, finding analogues, and building categories based on chemical and mechanistic similarity, and for predicting substance properties based on data from similar chemicals.
- The JRC **QSAR Model Database** (EC-JRC, 2024) is an archive providing information on the validity of QSAR models that were submitted to JRC's EU Reference Laboratory for Alternatives to Animal Testing (EURL ECVAM). It provides information on 154 QSAR models for various endpoints.
- The Danish EPA **(Q)SAR Database** (Danish EPA, 2024) is a collection of structural information and QSAR predictions, containing structural information for approximately 170 000 chemicals. It contains QSAR predictions for more than 40 endpoints.
- The US EPA **EPI Suite** (EPA, 2024) is a type of software that predicts various physical-chemical properties and environmental fate endpoints and also include models for environmental transport

This information can be completed with *in vitro* assays and *in vivo* studies in higher tiers, as more data is needed for the completeness of the assessment, and higher certainty is needed for a conclusive classification and assessment.

4.2.2 Hazard classification

The SSbD criteria for Step 1 build-up on the CLP criteria for the classification, labelling and packaging of substances and mixture. The CLP hazard classes and categories are split in the three groups introduced in the CSS and further defined in the Ecodesign Requirements for Sustainable Products (ESPR) (European Commission, 2022d): most harmful substances (H1), Substances of concern (H2) and other hazard classes (H3) (Caldeira et al., 2022a).

The framework sets an “early warning” for chemicals/materials that do not pass the H1 criteria. The purpose is to raise awareness (red flags) on certain aspects that the innovator should consider when innovating to prevent or anticipate future consequences and legal requirements. Chemicals and materials which do not pass the Criterion H1 in Step 1 should be:

- Prioritised for substitution
- (Re)designed to reduce their adverse effects
- Only allowed in uses proven essential for society (e.g. if their use is necessary for health, safety or is critical for the functioning of society and if there are no alternatives that are acceptable from the standpoint of environment and health)
- Safely used and their emissions/exposure controlled along the whole life cycle while activities are undertaken to develop alternatives as soon as possible; their use then should be phased out, once less hazardous alternatives are available
- Tracked through their life cycle

4.2.3 Hazard assessment

From the information, collected, generated, and evaluated, the assessor will derive the tolerable maximum level of exposure for the assessment in the following steps. These are the levels above which a particular human population (e.g. workers, consumers), the environmental compartments (soil, water, air) and the planetary boundaries (toxicity and ecotoxicity) should not be exposed.

These maximum levels are derived from the hazard endpoint by applying assessment or characterisation factors (protection factors) that quantify the effect of the chemical on a certain population or impact category. These values are compared against the predicted or measured levels of the chemical/material that exist, based on the fate properties and the use/exposure scenarios.

The Derived No Effect Level (DNEL) and the No Observed Adverse Effect Level (NOAEL) are the maximum levels above which a particular human population (e.g. workers, consumers) should not be exposed. These values may vary for specific (sub)populations, since some (e.g. children, pregnant women) require more protection than others, and for different exposure routes (oral, dermal, inhalation), and possibly also for different exposure scenarios (e.g. single exposure, short-term exposures, continuous lifetime exposure) (ECHA, 2011a).

The occupational exposure limits (OELs) are other types of maximum levels above which, in this case, workers should not be exposed and that can be used for Risk Assessment purposes. OELs are established at EU and national level, and are typically derived by independent scientific expert committees which consider available scientific information; they are complemented by information on exposure monitoring, such as sampling methodology, measurement methods and measurement systems. Note that OELs are not available for all chemicals and material.

Similarly, the Predicted No Effect Concentration (PNEC) is the maximum concentration of a substance above which a particular environmental compartment (e.g. soil, water, air) should not be exposed (ECHA, 2011a).

In Life Cycle Assessment (LCA), the Human Effect Factor (EF) is used to quantify the impact of emissions on human health. It represents the potential to cause adverse health effects in humans and is expressed in units that reflect the impact of emissions on human health, such as disability-adjusted life years (DALYs) or similar metrics. One DALY represents the loss of the equivalent of one year of full health.

4.3 Step 2 and Step 3: Safety aspects in the chemical/material production, processing, and final application.

4.3.1 Introduction

Understanding and estimating the exposure to a chemical/material is one of the fundamental requirements for safety assessment. Although it is not as extensively discussed as the hazard identification in the context of the SSbD framework, it is a key aspect in achieving both the CSS and the goals of the Green Deal related to strengthening the protection of human health and the environment. The assessment and the minimisation of the exposure to chemicals and materials plays a central role here.

To understand and estimate the exposure it is important to specify the use in which the chemical/material is utilised or applied.

Any activity for which there is a potential for human or environmental exposure to a chemical/material is defined under REACH (European Parliament and the Council, 2006) as “use”: use means any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, and production of an article or any other utilisation.

In addition, products are defined as any physical goods that are placed on the market or put into service. And substance on their own, mixtures, materials, articles, or complex products used by consumers, industrial or professional users are considered final products.

Therefore, a chemical/material can be a final product, or it can be used to produce the final product (while not being present in the final product itself) and/or it can be contained in the final product.

However, the SSbD strives to make a difference between those “uses” that can be regulated - and therefore better known and more manageable (e.g. occupational) - and those “uses” that cannot be regulated, and which may only be managed to a certain extent. Industrial uses are regulated, for example, by occupational safety and health (OSH) legislation and/or the Industrial Emissions Directive (IED) (European Parliament and the Council, 2010, as amended (revised I“ED 2.0” legislation to be published in 2024)) which set known high effectiveness requirements in risk management measures such as closed systems, ventilation and training. On the other hand, the safe use of consumer applications relies on the instructions of use based on information on consumer habits and practises. This distinction also tries to differentiate between those more generic uses (covered in chemical horizontal legislation, such as REACH and CLP) and product-specific uses (covered in vertical and product specific legislation such as that related to plant protection products, biocides, cosmetics, human and veterinary medicines, food contact materials (FCM), or toys, etc.). However, the line that separates these scenarios sometimes is diffuse, and it is not clear where a particular use should fall. In these cases, the assessor should make sure that the use is covered either in Step 2 or Step 3, and that all the relevant aspects for the particular safety assessment are covered.

Therefore, this section covers both Steps:

- Step 2 - Human health and safety aspects in the chemical/material production and processing phase
- Step 3 - Human health and environmental aspects in the final application phase.

4.3.2 Safety assessment

The safety assessment encompasses the identification, quantification, risk analysis (qualitative, semi-quantitative, and quantitative) and evaluation of risks associated within the SSbD system.

The key aspects of the safety/risk assessment are the hazard assessment (identification of the intrinsic properties and their effects), the exposure assessment (identification of the use and the prediction of exposure) and the risk characterisation (the estimation of the likelihood and severity of the effects).

The hazard assessment component of the safety assessment is covered by Step 1 in the SSbD and has been covered in Section 4.2., while the overall safety derived by the exposure assessment during the use (processing and application) of the chemical/material are covered in Steps 2 and 3 of the SSbD and in this section of the guidance.

4.3.2.1 Exposure identification and assessment

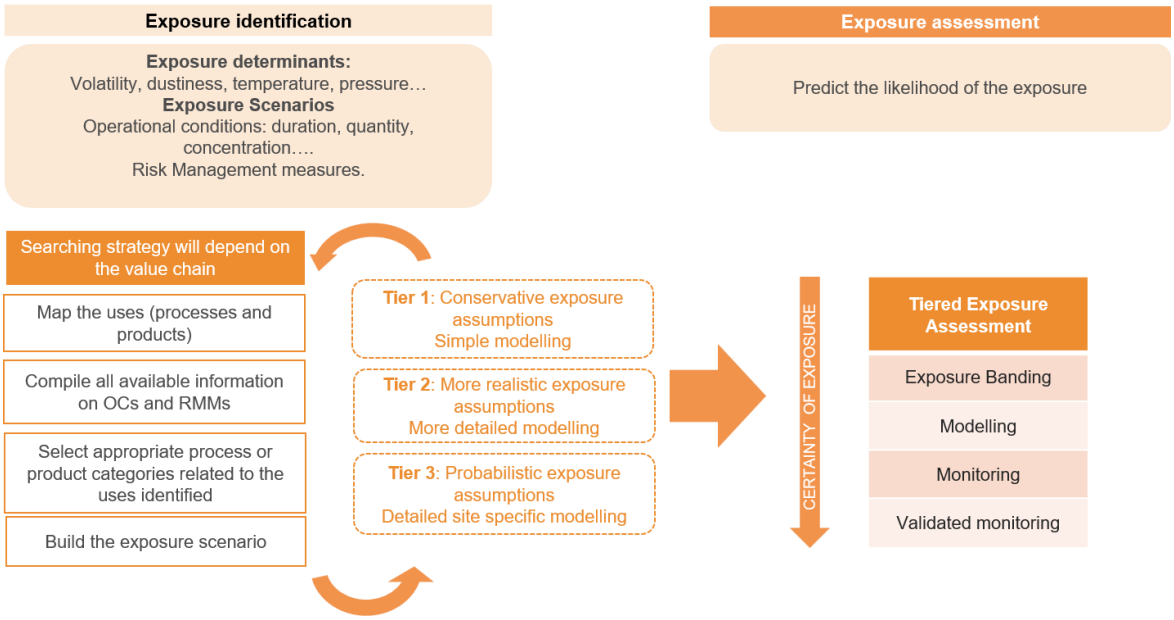
The exposure and safety assessment start with the identification of the use case. The use case describes scenarios that will raise a concern with regards to the safety to the human health and /or the environment. This is of paramount importance in safety assessment, because although the intrinsic properties of the chemical/material (hazard) remain the same during the entire life cycle, the exposure and therefore the risk will be specific to the use case.

The use case explains how actors in the value chain interact with the chemical/material in its life cycle (the SSbD system). It outlines the flow of actors’ inputs, establishing successful paths to implementing the SSbD framework.

It should be noted that the SSbD implementation is a multi-stakeholder effort and that therefore data and information should flow in both directions of the value chain. Also, the identification of the use case will allow actors to better understand the SSbD system and their role in it.

Relevant aspects for the exposure assessment and risk characterisation as described in this section are shown in Figure 13.

Figure 13. Scheme of the relevant aspects for the exposure identification and assessment. OC: Operational Condition, RMM: risk management measure



Source: Own elaboration

The basis for the exposure assessment is the exposure scenario. The development of the exposure scenarios starts with the mapping of the uses of the chemical/material, together with the processes and products in which the chemical/material is used.

This process will also help the assessor to have a better understanding of which of the "uses" fall into Step 2 or Step 3 of the SSbD.

The exposure scenarios identification will depend on the value chain, but should ideally consider the steps to:

i. Map the uses (see Section 3.2 for the definition of the SSbD system): analyses the market based on known information. Consider all potential uses beyond the immediate actor in the supply chain. Engagement with the entire value chain as early as possible in the research and innovation process and the implementation of the SSbD framework is recommended.

ii. Apply the standard descriptor system (ECHA, 2015) as appropriate (see Section 4.3.2.1.2)

iii. Compile all available information on (Operational Conditions (OCs) and Risk Management Measures (RMMs) related release/exposure levels during the life cycle of the substance (see Section 4.3.2.1.2)

iv. Select appropriate process or product categories related to the uses identified

v. Build initial exposure scenarios based on the input data needed for the Tier 1 exposure estimate, and make an initial exposure estimation and risk characterisation.

The process of gathering data is an iterative process that leads to collection of refined data and higher quality of available data. As more data becomes available, higher tier estimation tools can be used and more realistic scenarios and predictions will be obtained.

4.3.2.1.1 Exposure identification in early innovation

In early stages of innovation, one or more pieces of information regarding the use of the chemical/material under assessment are often missing. However, both for substituting a chemical/material and developing a new one, innovation nearly always takes place with a final product/application in mind. For example, if the intention is to substitute a phthalate plasticiser (the function of which is to soften a plastic material), we can already identify the product applications in which it is used, and for which substitution could be relevant, e.g. as a food contact material. If the idea is to develop a new material, its function is already defined (antimicrobial, flame retardant, etc.); therefore, the product/ type(s) of applications in which this functionality can be useful are, to a certain extent, already identified.

In this context, the use of the worst-case product or representative product is common practice in chemical risk assessment. The worst-case approach represents a frequent use of a product under unfavourable conditions and therefore its worst performance in terms of safety. This could be extended to R&I activities and also applied in the context of SSbD. For transparency and clarity, the selection of the chosen worst-case product should always be justified.

4.3.2.1.2 Exposure scenarios description

Any activity for which there is a potential for human or environmental exposure to a chemical/material is defined under REACH (European Parliament and the Council, 2006) as “use”: use means any processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, and production of an article or any other utilisation. Therefore, in the context of the SSbD it covers the chemical/material processing and the final product/application.

The description of the use(s) is based in multiple elements including the definition of the scenarios in which the exposure occurs, the technical functionality and the products that are placed on the market from the use in different value chains.

“Exposure scenarios” (ES) is the term introduced by REACH to describe the operational conditions and risk management measures that ensure that these uses are safe (the risk to human health and the environment is under control) during the life cycle of the chemical/material.

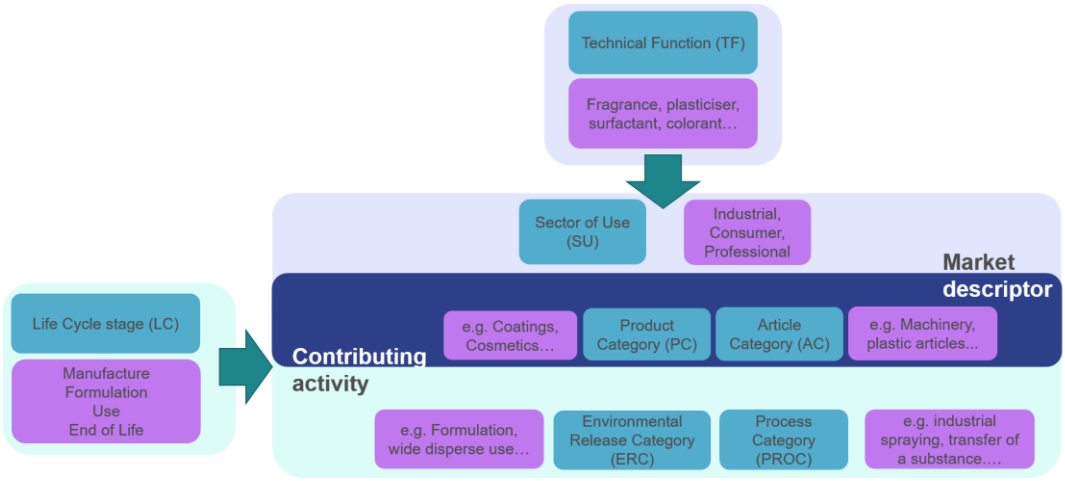
Exposure scenarios can include several contributing scenarios. A contributing scenario describes each contributing activity within an identified use, for example mixing, transferring into small containers, or applying a substance or mixture by spraying.

The uses are described by The REACH use descriptor (Chapter R.12), a system developed by ECHA to facilitate chemical risk assessment and supply chain communication. These descriptors aim to identify, describe, and communicate in a standardised format the different uses of a chemical/material life cycle stages. These descriptors have been also integrated in modelling tools such as the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Targeted Risk Assessment (TRA) and European Union System for the Evaluation of Substances (EUSES) and are used as input parameters to derive exposure estimates.

Regarding the SSbD system description, the logical way to describe the uses of a chemical/material is to structure them according to the life cycle. Each life cycle stage may consist of different uses. In addition, each use should be described with the following elements, see below. For each element, the

innovator could identify the information relevant for the ongoing innovation and system under assessment (Figure 14).

Figure 14. Overview of the descriptor system and information that they provide to the overall SSbD assessment



Source: Own elaboration

- **Life cycle stage (LC):** identifies the life cycle stage of the substance and includes the four basic steps or stages in its life cycle: the manufacture, formulation (including repacking), the end-use (including industrial use, professional use, consumer use), and (article) service life.
- **Descriptor list for technical functions (TF):** this element indicates the technical function of the chemical/material meaning what actually does in the use (e.g. solvent, pigment). The TF provides an idea of the kind of product/article and the sector in which the chemical/material will be used. However, the TF should be clearly distinguished from the Product Category (PC). For example, a substance can be used in anti-freeze products (PC4) without being itself an anti-freezing agent. It could be a colouring agent in the anti-freeze product.
- **The terms SU, PC and AC** (see below) provide information about the market in which the chemical/material is used
- **Sector of use (SU)** describes in which sector the chemical/material is used. This descriptor does not apply to consumer uses.
- **Product category (PC)** describes the types of chemical products in which a substance is used, the operational conditions and risk management measures to determine the level of consumer exposure.
- **Article Category (AC)** describes the type of article (including plastics and dried mixture) in which the substance has been processed.
- **Process category (PROC)** describes the application techniques or process types, the operational conditions and risk management measures to determine the level of occupational exposure for workers and professional users.
- **Environmental Release Category (ERC)** describes the broad conditions of use from an environmental perspective, based on those characteristics that give a first indication of the potential release of the substance to the environment. It determines the level of environmental exposure.
- PROCs, ERCs, PCs, and ACs provide information with regards to the contributing activities for exposure. And can be used as input parameters to derive exposure estimates in modelling

tools such as ECETOC-TRA. (European Centre for Ecotoxicology and Toxicology of Chemicals-Targeted Risk Assessment).

The guidance R.12 provides further guidance on how to assign the different use categories to the specific cases.

Besides describing the use, the operational conditions in which these uses take place need to be considered for the exposure estimation.

The ECHA Risk management measures and operational conditions (Chapter R.13) guidance provides supporting guidance on the most common types of use conditions having an impact on exposure. It includes an overview of operational conditions and risk management measures related to exposure of workers, consumers, and the environment.

Exposure estimation tools are especially used to support occupational safety assessments. The input parameters for the different worker exposure assessment tools largely address the same core exposure determinants. These are called "**core conditions of use**", core CoU, and they are the Conditions of use that are needed to run a Tier 1 exposure assessment with most of the exposure tools. The core CoU are:

- Percentage (w/w) of substance in mixture/article
- Physical form of the used product
- Duration of activity
- Occupational health and safety management system
- Room ventilation
- Local exhaust ventilation
- Respiratory protection
- Dermal protection
- Face and Eye protection
- Place of use
- Operating temperature

4.3.2.1.3 Exposure prediction/ assessment tools

The identification of the exposure scenarios, together with the description of the operational conditions/use conditions, provide the information to predict the exposure potential that can be minimised to ensure safe use by applying risk management measures.

Exposure models also provide the means for predicting chemical/material levels at a specific point in time, in a specific medium and therefore the potential of exposure for human health and the environment. To make their use more practical, models are often integrated into tools with a user-friendly interface.

Exposure Models Working Group of the European Chapter (ISES Europe) produced a mapping of relevant available models and tools for exposure assessment. The aim is to provide guidance to enhance transparency of choices made in the selection of models, tools, and exposure-related input data and to better understand the quality of model results. The mapping covers:

- **Workers** with tools and models for exposure assessment of occupational exposure due to handling of chemicals at workplaces

- **General population** (humans) with tools and models for exposure assessment of humans via the environment and for exposure assessment due to handling of chemicals by consumers (including different sub-populations)
- **Environment.** (ecosystem) with tools and models for exposure assessment of environmental compartments due to emissions to the environment.

The innovator can benefit for the mapping and evaluation done by ISES members and identify the most appropriate tool to be used based on some descriptors like those shown in Table 3 (Schlüter et al., 2022).

Table 3. Examples of the information on the models and tools collected for the mapping

Descriptor	Explanation of the descriptor
Exposure target	The human (sub)population (consumer, worker, general population) or environment (compartment)
Route of exposure	Route of exposure for humans (inhalation, dermal, oral) or environmental compartment (water, soil, air)
Sources of exposure	Activity or material where the substance is released or emitted and leads to exposure
Product class/chemicals/substances	Type of chemical (substance, mixture…), product class (cosmetic, pesticide…), form (vapour, particle…)
Tier/complexity:	Classification of use of the tool regarding complexity, and if applicable characterisation into tiers used in regulatory exposure assessment (tier 1-screening tool, tier 2-more complex, tier 3)

Source: Own elaboration adapted from Schlüter et al., 2022.

4.3.2.2 Risk Characterisation/assessment

The risk is characterised as a combination of the chemical/material hazards characterisation and the exposure assessment to the human health and the environment (Figure 15).

For characterising the risk associated to the use the assessor should:

II. Establish the significant routes of exposure and a first estimate of expected exposure levels. Compare any known exposures and/or the predicted exposure with the available toxicological knowledge from the hazard assessment in a risk characterisation.

III. If the available data indicate that for certain uses the risk is too high, e.g. the DNEL/NOAEL values are exceeded, further refinement is needed either of the hazard assessment or of the exposure assessment (or both).

IV. Decide whether:

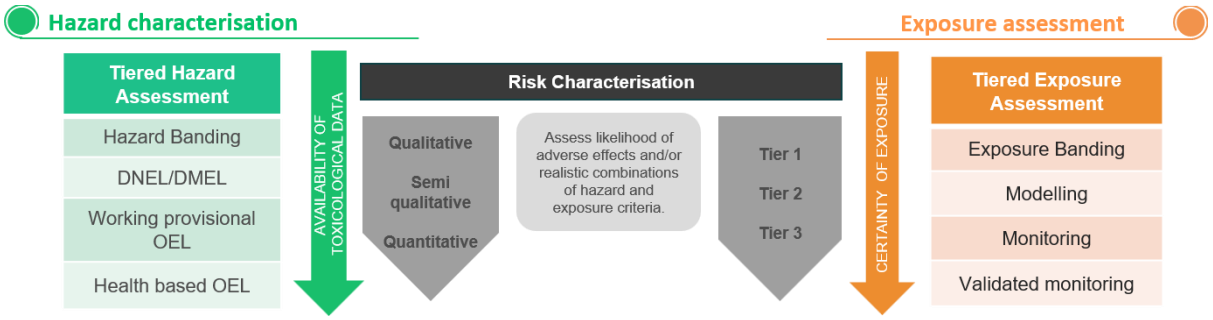
  (a) Hazard further testing is needed, identify the data needs, propose a testing strategy (go to Section 4.2.1

  (b) Exposure: measured data or a higher tier model is needed. Apply another model or use measured data to i) refine the exposure scenario and ii) demonstrate control of risk. (Go to Section 4.3.2.1

V. Carry out further exposure assessment and risk characterisation

VI. Conclude the exposure estimation and risk characterisation (including uncertainty analysis):

Figure 15. Relevant aspects for the risk characterisation



Source: Own elaboration

As in the case of hazard characterisation and exposure estimation, risk characterisation is an iterative and tiered process that will progress hand in hand with the two different and integrative components of the assessment.

Depending on the approaches used, and the available data derived both from both the hazard and exposure assessment, it will be also possible to perform the risk characterisation in a tiered approach, ranging from a qualitative (i.e. lowest tier) to a quantitative characterisation as data becomes available.

The following refinement options are available, depending on what the assessor considers to be the most efficient strategy.

- *Improving the hazard information*
- *Improving the exposure information*
- *Improving information on operational conditions*
- *Improving information on risk management*

The quickest and most cost-effective approach is to improve the realism of the exposure and risk management assumptions of the assessment.

If sufficient exposure information is available, more complex exposure models ('higher tier' models) may be employed to get a more precise exposure estimate. Running such models would normally require the collection of additional information related to the use and use conditions.

Uncertainty analysis can be used in the iterations to test the robustness of the risk characterisation, to identify the most uncertain inputs to the entire assessment (whether hazard or exposure related) that influence the risk characterisation, and thereby to decide on the most cost-effective way to collect any additional information needed on these elements to improve the assessment.

In some cases, the safety assessment may lead to the conclusion that certain types of uses can no longer be supported.

4.4 Information sources

Communication of information up and down the supply chain is very important to ensure the safe use of chemicals and materials throughout their entire life cycle. Safety Data Sheets are a globally recognised tool and are widely used for communicating information on chemicals and materials in the supply chain. Other tools, such as Exposure scenarios and use maps, have been newly developed in the context of specific legislation for the communication of uses. Innovators can leverage these existing

tools to retrieve relevant information for their specific chemicals and materials and their uses. They may well develop and extend them further for particular R&I activities.

Extended Safety Data Sheets

Safety data sheets include information about the properties of existing chemicals, hazards and general instructions for handling, disposal, and transport and first-aid, firefighting, and exposure control measures.

The SDS information may be extended by exposure scenarios, which include specific information on how the exposure of workers, consumers and the environment to hazardous substances can be controlled during the specific uses identified.

This type of information can be useful to retrieve information with regards to existing chemicals/materials like the hazard classification, the occupational exposure limits and/or data related to their intrinsic properties.

Exposure Scenarios

Exposure scenarios summarise the key information contained in the chemical safety assessment, to ensure its safe use. They describe how to control the exposure to the chemical concerned of workers, consumers, and the environment, based on input parameters describing the conditions of use and the risk management measures.

An exposure scenario describes the use based on the REACH use descriptors, the conditions of use affecting the exposure, the exposure estimation ensuring the safe use and guidance to evaluate that the use is performed following these boundary conditions.

This information can be useful when substituting an existing chemical/material for an identified use or when improving the OC and RMMs. It can also support the innovator by providing real examples on how to define exposure scenarios and how to use REACH use descriptors for the identification of its own use.

Use Maps

Similar information can be retrieved from the use maps, with the difference that while the exposure scenarios are provided for specific chemicals/materials, the use maps provide this information for the common uses in a specific sector.

The “use map” concept was developed to improve the quality of information on use and conditions of use communicated up the supply chain, and likewise to improve the efficiency of this communication process.

Use maps are typically generated by downstream user sector organisations, via collecting information on the uses and the conditions of use of chemicals in their sector, in a harmonised and structured way. For this purpose, the “use map package” was developed under the CSR/ES Roadmap.

The use map gives an overview of the common uses in a specific sector using the **REACH use descriptor system**. Each use consists of several contributing activities that are also listed. For each contributing activity, a link is provided to the corresponding exposure assessment input parameters. The input includes the **conditions of use and risk management measures**, and it is provided for workers’ exposure assessment (SWED), consumers’ exposure assessment (SCED) and/ or environment exposure assessment (SPERC).

The Use maps library (ECHA, 2024) currently includes use maps developed by the following organisations:

- AISE International Association for Soaps, Detergents and Maintenance Products
- CEPE European Council of the Paint, Printing Ink and Artists' Colours Industry
- CLE CropLife Europe
- Concawe Fuels
- Cosmetics Europe Cosmetics and personal care products
- EFCC European Federation for Construction Chemicals
- ESIG European Solvents Industry Group
- EuPC European Plastics Converters
- FEICA Association of the European Adhesive and Sealant Industry
- Fertilizers Europe
- I&P Europe, Imaging, and printing products Europe
- IFRA International Fragrance Association

The use maps templates are available to develop or update use maps by sector organisations. This harmonised practice could be extended to other kinds of chemicals/materials and product/applications. The SSbD can both benefit from use maps library to retrieve relevant information but also to develop new use maps.

ConsExpo factsheets

A similar concept to the use maps can be found in the ConsExpo factsheets. In this case the information is not linked to the REACH use descriptors but to ConsExpo.

ConsExpo is a modelling tool that can be used to estimate consumer exposure to a wide variety of products in a wide variety of circumstances.

The fact sheets are documents presenting information important for the consistent and harmonised estimation and assessment of the exposure to substances from consumer products when using ConsExpo Web (RIVM, 2024a).

In the fact sheets, information about exposure to chemical substances is compiled for certain product categories, and default parameters are given. These fact sheets describe various exposure scenarios for the specific products and set defaults for relevant exposure parameters. The fact sheets have been developed for characterising and standardising the exposure estimation, in combination with the ConsExpo Web tool.

The ConsExpo tool is based on default parameters provided in the fact sheets that represent the most conservative reasonable worst-case scenario, i.e. one which represents consumers who frequently use a certain product under unfavourable conditions.

The factsheets are also useful for any exposure estimation without the use of related exposure related software. They provide general background information that can be very useful in R&I, and likewise in the context of the SSbD.

The following fact sheets have been developed and are currently used in the ConsExpo model (RIVM, 2024b):

- General Fact Sheet
- Air Fresheners Fact Sheet

- Cleaning products Fact Sheet
- Cosmetics Fact Sheet
- Disinfectant products Fact Sheet
- Do-It-Yourself products Fact Sheet
- Paint products Fact Sheet
- Pest control products Fact Sheet
- Children's toys Fact Sheet (defaults from this fact sheet are not included in the ConsExpo Web database).

RMM library

At the start of the REACH implementation, the European chemicals trade association, Cefic, set up a library of RMMs, containing a first structured collection of available RMMs for the different target groups and exposure routes in exposure assessment. This library addresses the control of exposure to consumers, environment, and workers. The information in the library relates to sectors, product groups, processes, or single horizontal measures like personal protective equipment (PPE).

The RMM library is an EXCEL spreadsheet that contains:

- A practical guide to use the library
- The library containing RMMs / OCs and details of their effectiveness; and
- Lists of information sources for consumers, environment, and occupational measures.

Corresponding to the library, ECHA published the Guidance Chapter R.13, providing an initial concept on how to define risk management in the context of a REACH exposure assessment, in turn providing additional guidance on the RMM library (ECHA, 2012).

A further developed library, the Integrated Risk Management Measures Library (ECEL 3.0) is available at the TNO's (Netherlands Organisation for Applied Scientific Research) Diamonds platform (CEFIC, 2024).

4.5 FAQs for the implementation of Step 1, Step 2, and Step 3

(Q)SAR models do not have a formal validation process, can I still use them?

The SSbD framework promotes and supports the use of any new scientific and technological development that can contribute and support its implementation. However, the SSbD does not set any specific criteria or requirements for these. The specificity and requirements will increase as the innovation evolves and gets closer to potential/future regulatory requirements.

Guidance is available for (Q)SARs. In particular, a (Q)SAR model may be considered valid if it is assessed in accordance with the OECD QSAR Assessment Framework. (Q)SARs can be an effective and efficient tool during innovation to initially identify "red flags", to guide innovation and be coupled with other information to be used in a weight of evidence approach.

What is the meaning of the H1 criteria in Step 1?

The purpose of the hazard-based H1 criteria in the context of Step 1 of the SSbD is to raise awareness on certain aspects that the innovator should consider when innovating to prevent or anticipate future consequences and requirements. Chemicals and materials which do not pass the Criterion H1 in Step 1 should be:

- Prioritised for substitution
- (Re)designed to reduce their adverse effects
- Only allowed in uses proven essential for society (e.g. if their use is necessary for health, safety or is critical for the functioning of society and if there are no alternatives that are acceptable from the standpoint of environment and health)
- Safely used and emissions/exposure be controlled along the whole life cycle while activities are undertaken to develop alternatives as soon as possible and their use is phased out as soon as less hazardous alternatives are available
- Tracked through their life cycle

What is the difference between Step 2 and 3?

In the context of Risk Assessment any activity for which there is a potential of exposure for human or environmental exposure to a chemical/material is defined is defined as "use", regardless of the type of target that is potentially exposed.

However, the SSbD strives to make a difference between those "uses" that are regulated and therefore known and manageable, and those "uses" that are unknown and cannot be managed.

This distinction also tries to make a distinction between those more generic uses (covered in chemical horizontal legislation such as REACH and CLP) and product-specific uses (covered in vertical and product specific legislation like Food Contact Materials, Toys, etc).

However, this line that pulls apart these scenarios sometimes is diffuse, and it is not clear where a particular use should fall. In these cases, the assessor should make sure that the use is covered either in Step 2 or Step 3 and that all the relevant aspects for the particular "use" are covered.

Is the environmental assessment also covered in Step 2 or only in Step 3?

The same justification applies to the environmental risk assessment. In industrial sites, the exposure to the environment is covered by directives such as the Industrial Emissions Directive, the Waste Framework Directive or the Water Framework Directive while activities outside industrial installations are arguably not as well controlled. Therefore, the higher impact to the environment is foreseen in activities covered in Step 3 in the framework. How-

ever, environmental considerations and assessment should be included in all uses where there is an exposure to the environment.

5 Step 4: Environmental Sustainability Assessment

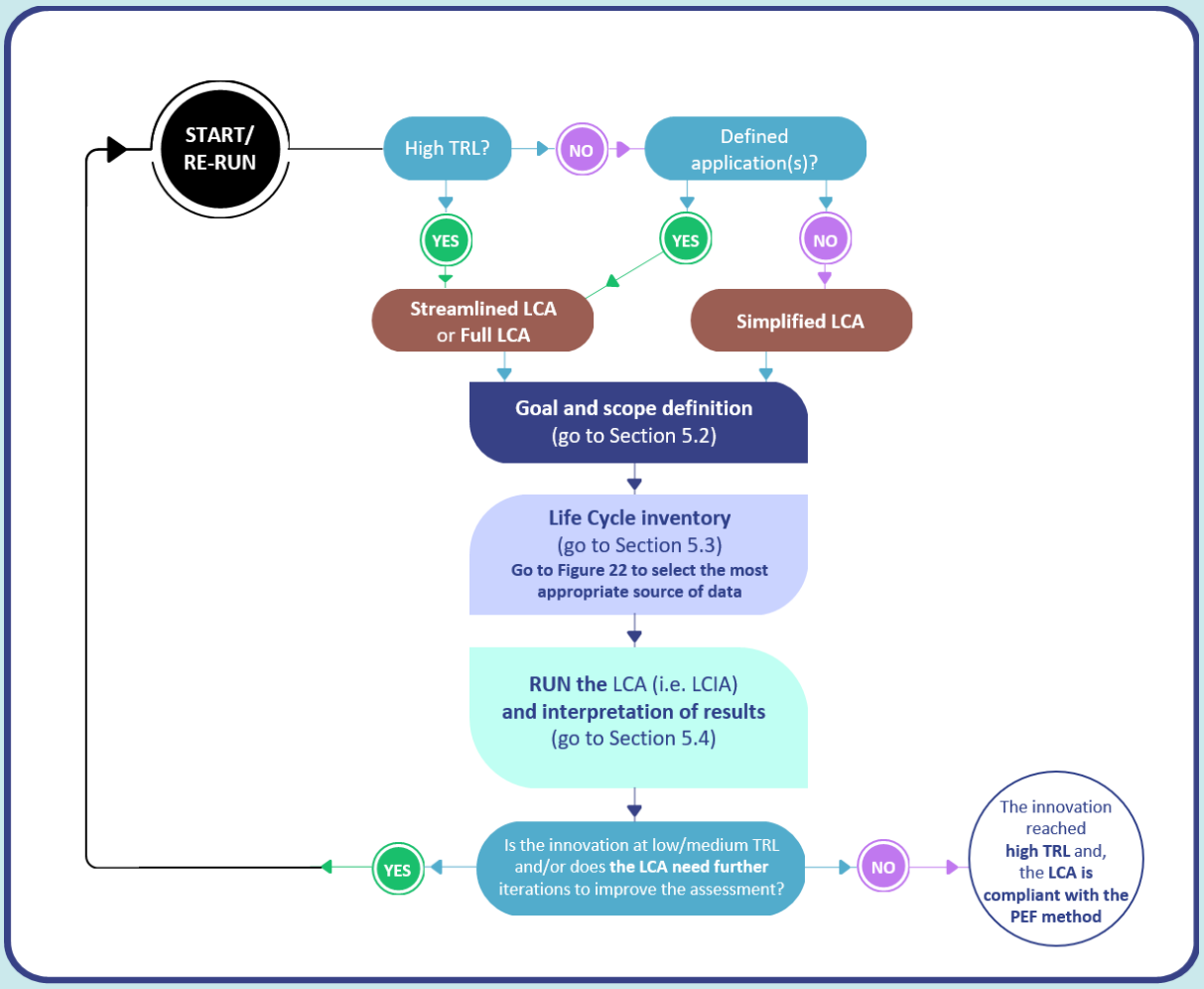
AIM OF THE SECTION:

This section gives an introduction on performing Life Cycle Assessment (LCA) with reference to the Technology Readiness Level (TRL) and associated level of data available. It guides the user on performing a tiered LCA according to the maturity of the innovation, including:

- **Narrowing the system boundaries (under specific conditions),**
- **Data generation and collection; and**
- **Interpretation of results to guide innovation**.

Adjustments to the described tiered LCA might occur over progressive refinements.

STRUCTURE OF THE SECTION:



Source: Own elaboration

5.1 Terminologies and background information to read the section

The inclusion of a LCA approach, during the innovation process, can be beneficial **to quantify the impact of the design goals and design principles implementation, and the (environmental) hotspots for further improvement**.

For the fundamental full knowledge and terminology commonly referred to in LCA methodology and regarding the Full LCA Product Environmental Footprint (PEF) method, the documents are freely available online: European Platform on LCA | EPLCA (europa.eu) (European Commission, 2024). Additional terminology used in this Section refers to the "tiered" type of LCA.

Here, this refers to progressively refining the LCA over iterations, related to both the data obtained and the level of assessment undertaken, each progression being a successive "Tier", as explained below:

- **Innovation technology:** all the innovation in the scope of the SSbD, for instance, chemical/material innovation, chemical/material substitution, or chemical/material-related process and product improvements.
- **Prospective** LCA: an LCA methodology suitable to new innovation processes, which estimate the associated environmental impacts before the new/ redesigned chemical or material is placed on the market, i.e., referring to ex-ante evaluations.
- **Tiered** LCA: this is the overall approach applicable in the context of the SSbD framework, so called because it comprises the progressively more developed LCA tiers of: a simplified LCA, a streamlined LCA and finally a full LCA.
- **Simplified** LCA: it is the full LCA with several assumptions and simplification due to some unknown aspects.
- **Streamlined** LCA: it comprises the iterative modelling of the LCA that goes from a simplified LCA to a more complete assessment but lacking the full detail of a PEF-compliant LCA or equivalent.
- **Full** LCA: it refers to an LCA that follow the recommendation in the PEF.

5.2 Goal and Scope Definition

The Goal and Scope definition in the LCA is complementary to the Scoping analysis performed for the definition of the SSbD system, by considering additional information to perform the Step 4. For further guidance regarding the Scoping analysis, go to Section 3.

5.2.1 General structure of the tiered LCA

Step 4 follows the PEF, which is the recommended method by the European Commission. During the process of innovation, the following constraints and aspects should be considered, to frame the LCA alongside the innovation stages of a chemical/material:

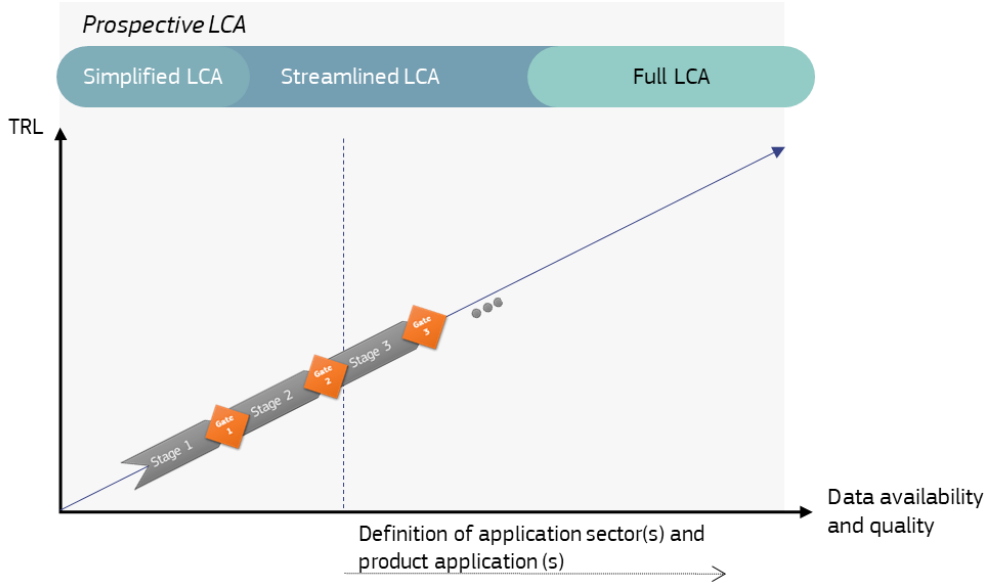
- The *knowledge of the innovation technology* - this will increase as the innovation proceeds. Initially, in the immature innovation stages, it is usual to have to consider, for instance, narrower system boundaries, the consideration of fewer impact categories, or make assumptions in the data used (e.g. the use of proxy data), using more limited (generic) data sources, and lower quality data.

- The *temporal scale* (timeline) between the start of the innovation and the placing of the end-product of the innovation process on the market. This needs to be reflected in the background data used to correctly include foreseen future changes of external aspects (e.g. changes in the electricity mix). Sacchi et al. can be used as an approach to include the temporal scale in the assessment (Sacchi et al., 2022).

These aspects affect the four steps of a ISO-compliant LCA (i.e. Goal and Scope definition, Life Cycle Inventory (LCI), Life Cycle Impact Assessment (LCIA), and Results Interpretation) (ISO, 2020), and should be reflected in the assessment, accordingly.

The Figure 16, shows how the tiered LCA is framed alongside the innovation stages of a chemical/material, which is represented by the stage-gate method. Table 4 provides and overview of the main aspects.

Figure 16. Tiered approach of the increasing completeness of the (prospective) LCA (referring to the dark grey area)



Source: Own elaboration

Table 4. Summary of the main aspects for the goal and scope definition to create a tiered approach for the LCA

Tiered LCA	**Simplified LCA**	**Streamlined to Full LCA**
Applicability	○ Usually low TRL ○ Data from laboratory ○ Un/Defined application(s)	○ Increasing TRL ○ Data from industrial or pilot scale ○ Defined application(s)
Main characteristics	▪ A Simplified LCA helps to identify the most important life cycle stages and processes for data refinement, and thus guide the optimal use of effort and re-sources ▪ Knowing the product or sector application of the chemical/material under development, it is possible to create scenarios describing the possible variabilities, for instance in terms of geography or products.	▪ Continuous iterative adjustment of the simplified LCA modelling, which follows the increasing maturity of the innovation. ▪ Examples of refinement include primary data collection, filling in data gaps, inclusion of all the impact categories, and expanding the system boundaries to cradle-to-grave (as opposed to cradle-to-gate) ▪ Effort regarding the collection of primary data for LCI via in-house data collection, enhanced engagement with suppliers and/or downstream users, making specific data requests, etc.

Tiered LCA		Simplified LCA	Streamlined to Full LCA
Goal and scope definition			
Functional Unit (see Section 0)	*Defined application*	As in PEF definition	
	Undefined application	Unit mass of the chemical/material (i.e. declared unit)	As in PEF definition
System boundaries (see Section 5.2.3)	*Defined application*	Cradle-to-grave, OR Cradle-to-grave *with scenarios* (if multiple application sectors are considered)	
	Undefined application	Cradle-to-gate	Cradle-to-grave OR Cradle-to-grave with scenarios (if multiple application sectors are considered)
Benchmark or Representative product (see Section 5.2.4)	*Defined application*	Definition of the representative product. If not available, definition of a product best representing the comparison	
	Undefined application	Not possible in most cases. Where the innovation consists of a substitution, use the chemical/material under substitution	Once the application is known, definition of the representative product. If not available, definition of a product best representing the comparison
LCI (further guidance in Section 5.3)		○ Data generation supported by laboratory tests ○ Scenarios reflecting different potential product applications	○ Effort needed to collect primary data for LCI via enhanced engagement with suppliers and/or downstream users, making specific data requests ○ Scenarios reflecting different potential product applications
LCIA (further guidance in Section 5.4)	*Defined application*	Narrowed to the most relevant environmental aspects (potential outcome of the Scoping Analysis – see Section 3.5)	As for the SSbD framework (Caldeira, C. et al., 2022a)
	Undefined application	Narrowed to the most relevant environmental aspects (potential outcome of the Scoping Analysis – see Section 3.5)	As for the SSbD framework (Caldeira, C. et al., 2022a)

Source: Own elaboration

5.2.2 Functional Unit

According to the PEF method (Zampori & Pant, 2019) (and general ISO-compliant LCAs), the Functional Unit (FU) defines the qualitative and quantitative aspects of the function(s) and/or service(s) provided by the product being evaluated. The Functional Unit definition answers the questions regarding the extent of the function or service ('what?'), the quantity of the function or service ('how much?'), the expected level of quality ('how well?'), and the duration/lifetime of the product ('how long?') (e.g. the Functional Unit of paint could be described as providing protection of $1m^2$ of substrate for 50 years with a minimum 98% opacity).

Simpler definitions of the Functional Unit can be provided when conducting a simplified LCA (see Table 4). In these cases, the Functional Unit usually reflects the unit mass of the chemical/material (i.e. declared unit). See the example in Box 2.

In the tiered LCA, it is important to note that *the Functional Unit may change along the innovation process* because of the increasing knowledge of the chemical/material under assessment.

5.2.3 System boundary

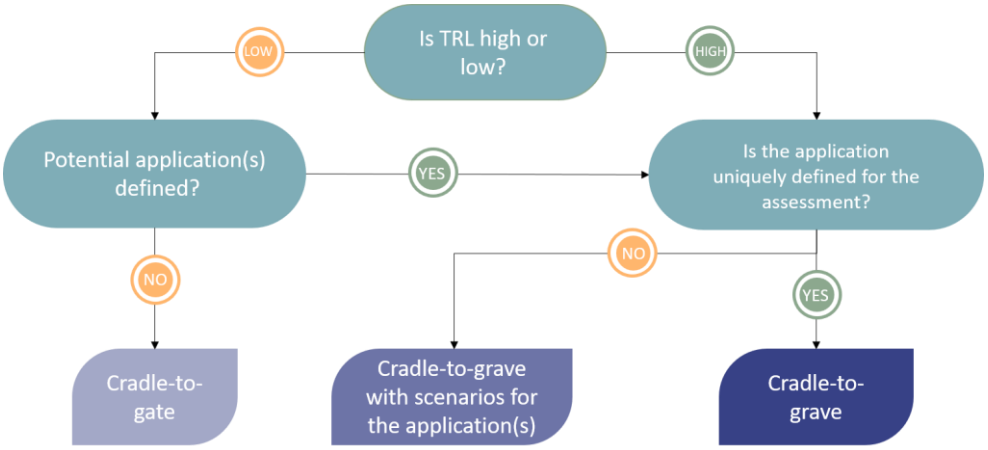
The system boundary can be defined following the decision tree in Figure 17, depending largely to the Technology Readiness Level (TRL). The definition of the "low" or "high" TRL is self-assessed according to the particular situation.

The simplified LCA could consider cradle-to-gate boundaries ONLY when potential applications are not yet well defined. When the potential applications are defined, it is always possible to consider the entire life cycle (cradle-to-grave) of the chemical/material by considering different scenarios for the different uses and/or EoL options. Narrower system boundaries can still help to identify hotspots in the production and manufacturing process of the chemical/material, as well as its precursors.

It is important to develop a cradle-to-grave assessment as soon as it is feasible, i.e., once it has been possible to define the application sector(s) and product(s). It is strongly recommended to perform a cradle-to-grave assessment as early as possible, because this comprises a more complete definition of the overall system boundary to then avoid the possibility of inadvertently shifting environmental burdens between life cycle stages or processes. This holistic assessment guarantees, as far as possible, that impacts are considered throughout the entire life cycle.

When multiple application sectors are envisioned, it is recommended to use scenarios to represent the possible alternatives. For each alternative, a cradle-to-grave LCA is necessary. Further advice on how to set the system boundaries accordingly are provided in Section 5.2.3.1.

Figure 17. Decision tree for the definition of the system boundaries. The choice of the system boundaries depends on the knowledge regarding the final application of the chemical/material under assessment



Source: Own elaboration

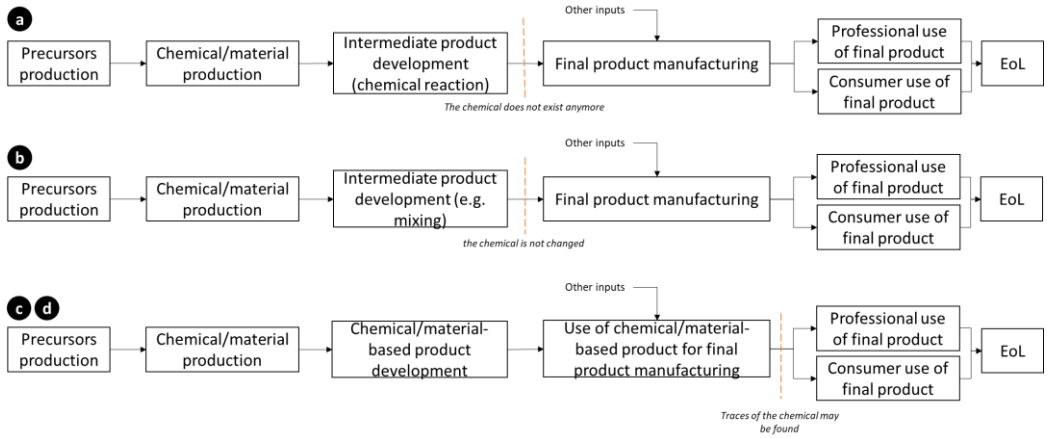
5.2.3.1 Chemical under assessment over its whole life cycle

The system boundaries for the chemical/material life cycle should reflect the use of the chemical/material and its purposes. According to the reason for using the chemical/material, the structure of the life cycle can be built in different ways, i.e., related to its end-purpose. Figure 18 shows the system boundaries for each of the above-mentioned purposes. The following possibilities are considered in the figure: a) a chemical/material used as a reactant in the production of the final product (i.e. does not exist as a separate chemical substance post-reaction); b) a chemical/material is physically combined with other chemicals/materials in the production of the final product (e.g. through mixing); and c) and d) a chemical/material is used in the manufacturing of the final product and is not meant to be part of the final product (with/without trace in the final product).

For instance, a chemical/material may be used to produce auxiliaries (auxiliary inputs) of materials or chemicals, which are then subsequently used to manufacture the final product(s). In other cases, the chemical may be a reagent (actively involved in the chemical process), and hence may disappear during this process, and be completely absent in the final product of the reaction. All these possibilities can affect the system boundary of the assessment.

This should be clearly stated in the definition of the system boundary, also in line with Steps 2 and 3 of the SSbD assessment.

Figure 18. Examples of the system boundary for the life cycle of a chemical/material according to its purpose



Source: Own elaboration

5.2.4 Selection of the reference/ benchmark

Usually, LCA defines a product to be used as a basis for comparison with all products having the same function (via adhering to the definition of a common Functional Unit, as previously discussed). Many ways of defining a benchmark can be used, depending on the goal of the comparison, all of which are underpinned by the assumption that these products have a similar function for end users and can substitute each other, and are therefore comparable over the entire life cycle. This is explicitly required both by ISO 14040 and 14044 and by the PEF methodology (ISO, 2006, 2020; Zampori & Pant, 2019).

In the SSbD context, often the innovation processes address a specific need, such as the substitution of an undesired chemical/material in one or more applications or finding alternative processes to synthesise a chemical to reduce the associated environmental impacts. In such cases, **the reference chemicals and application can be used as a reference for the innovation process, keeping in mind that the two systems must be compared based on the stipulated functionality.**

In this sense the comparison will answer the question "Can the newly developed chemical/material provide the same function as the reference chemical/ material, but with lower environmental impacts throughout its entire life cycle?"

If the goal of the innovation is to place a new chemical on the market, without the goal of substituting a specific chemical, but rather to compete against a set of other options, then a more suitable approach could be the **definition of a "representative product", to be used as reference, as provided in the PEF method**. In this case, **an "average chemical" (as the representative product) can be defined, if one knows the market share of each relevant chemical for the intended application**. Then, the relevant environmental performances of such representative products are used as a reference to for the comparison, answering the question: "Can the newly developed chemical/material provide the same function of the competing chemical/ material, but with an environmental impact that is lower than the market average?" Considering the relevance of the choice of a reference chemical or material for the final results, it is paramount that the choice is duly motivated and communicated in a transparent manner.

Box 2. Example of the Goal and Scope definition of the innovation process of a chemical/material

The present example is provided to explain how the definition of the goal and scope for the LCA need to be revised and refined along the innovation process. The definition starts from the goal of the innovation that in the example is *"(re)design a plasticiser with renewable resources".* The material that should help the fulfilment of the innovation goal is currently under development (i.e. low TRL). Figure 19 illustrates the information regarding the Goal and Scope definition along the innovation.

The material must have specific functional characteristics. At this point, a range of application sectors is known, but not defined, and neither is the specific product defined. Hence, a cradle-to-gate assessment is performed. With this system boundary, the functional unit is defined as the mass unit of the material (i.e. declared unit).

Once the assessment has been performed, and the results are obtained and used for further development, the material development reaches in parallel a higher TRL. The goal of the innovation might then become more specific, e.g. *"(re)design a plasticiser for concrete in building construction".* At this point, the application has become well defined. This requires a refinement of the Functional Unit, as well as the system boundaries, and the criteria considered also based on the selected product and the expected characteristics according to the desired performance.

The example emphasises how the definition of the Goal and Scope may change along the innovation process, following the increasing awareness and knowledge of the innovation itself, which would at the end include the final application. The new functional unit would then reflect the changed, better-known functionality of the final product (containing the chemical/material under assessment as an "ingredient"). **This means that the role of the chemical/material itself should not be explicitly mentioned in the functional unit. However, the presence of the chemical/material under development will affect the performance of the product application as well as the environmental impact**.

Figure 19. Example of the Goal and Scope definition of a chemical/material

Goal of the innovation	(Re)design a plasticiser with renewable resources	Concrete for building construction with the (re)designed plasticiser
Innovation stage	Low TRL	High TRL
Known application	No	Yes
Collected characteristics	Material-specific characteristics (viscosity, density, etc.) + characteristics linked to the goal of the (re)design	Application-specific characteristics of the material for the desired performance + amount of the material to fulfill the goal
Functional unit	Amount of material (i.e. declared unit)	m3 concrete with X% of workability and durability
System boundaries	Cradle-to-gate Gate-to-gate	Cradle-to-grave (of the concrete containing the plasticiser)
Impact categories	Literature review identifies relevant impact categories (e.g. Resources, climate change, Land use, others..	All the impact categories

Source: Own elaboration

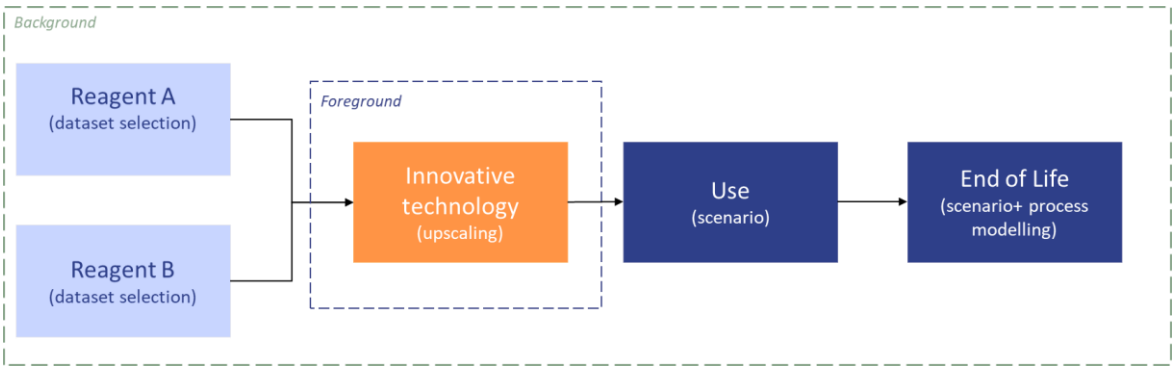
5.3 Life Cycle Inventory: Data generation and collection

The LCI includes all the material and emission flows along the entire life cycle of the chemical/material under assessment. Guidance to generate the LCI is provided by the PEF method. This section provides **additional guidance for the generation and collection needed to perform the tiered LCA, i.e. in the context of the chemical/material innovation**. Figure 20 shows a general scheme of a chemical/material life cycle. Starting from the innovative technology under assessment, there are upstream and downstream processes to complete the life cycle.

From a data point of view, in LCA (and in Social LCA as described in Section 6.1.1), the system is split in background and foreground system. The innovative process is considered as the *foreground*[1] *system*; while the upstream and downstream processes are referred to as the *background*[2] *system*. The upstream processes include the processes related to the acquisition of the reagents or precursors needed for the innovative process; the downstream processes can be summarised into the set processes where the innovated chemical/material is used. The last part of the life cycle is the end-of-life of the chemical/material.

The use and the end-of-life life cycle stages might not be known if the innovative process has a very low TRL (see Section 5.3.3). For this reason, the figure shows the scenarios that are needed to complete the assessment. More specific guidance is provided for the foreground and the background systems here below in the dedicated subsections 5.3.1 and 5.3.2.

Figure 20. Example of different strategies for data collection and generation for different stages of the life cycle



Source: Own elaboration

[1]It includes all the processes that can be directly studied, and for which specific data can be collected. Therefore, it includes the activities carried out by the company performing the assessment and as well as direct suppliers or users for which it is possible to collect the data.

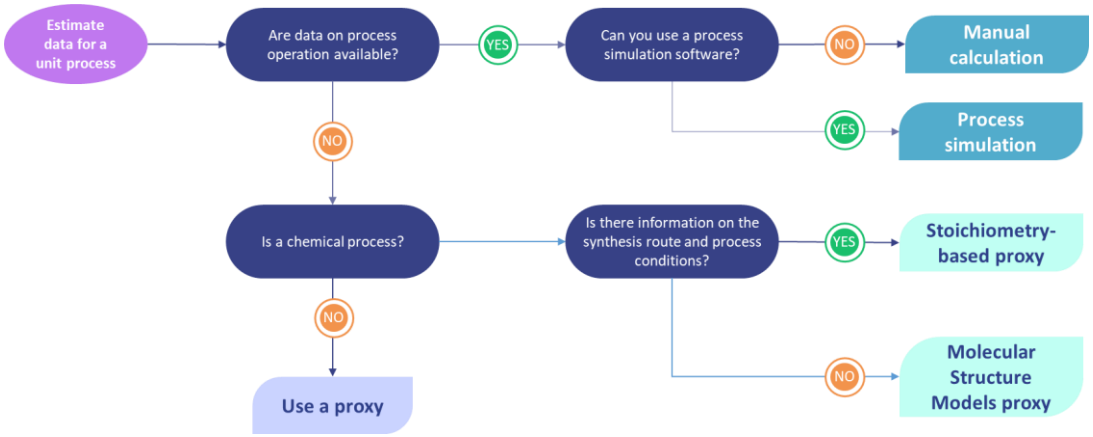
[2] It includes further upstream or downstream processes in the product system, for which generic data from databases can be applied).

5.3.1 Foreground system

The LCI of the innovative technology under assessment (i.e. the foreground system) is iteratively updated throughout the innovation process. The iteration will follow the increasing quality and representativeness of the data.

Compared to a full LCA, in the tiered LCA for a chemical/material under development, there are the following two main constrains regarding consumption and emission flows: (1) these might not be known; (2) when collected at laboratory scale, they do not represent the production of the innovative technology at the industrial scale (i.e., as the process becomes more commercially viable, there are usually built-in "economies of scale"). Based on these two points, a decision tree is proposed in Figure 21, based on existing studies (Parvatker & Eckelman, 2019; Tsoy et al., 2020). This is proposed to navigate among the different strategies, to upscale processes or to choose proxy data.

Figure 21. Decision tree for the selection of the data sources for the data collection and generation. Decision tree adapted from (Parvatker & Eckelman, 2019; Tsoy et al., 2020)



Source: Own elaboration based on Parvatker & Eckelman, 2019; Tsoy et al., 2020.

- **Manual calculations**: Piccinno *et al.*, 2016 provided easy equations or default values for the most popular chemical processes in laboratory scale (e.g. heating systems) to scale the process at industrial scale. This approach can be useful to derive some key data for a simplified LCA (e.g. mass and energy balances) of the process developed.
- **Process simulation**: a more refined approach compared to the previous one is to use software that can simulate chemical and physical processes. They can be utilised to estimate more accurately input and output flows to the process that can be then used in compiling an LCI.
- **Use of a proxy**: When data for a specific chemical or material is not available, a different chemical/ material may be used, to estimate the impact of the missing (actual) chemical/ material. This choice has to be made very carefully, paying attention to the similarities and differences in the life cycle of the desired chemical/ material and its proxy. In particular, it is important to check the technology(ies) in the supply chain and the relevance of the dataset in the analysis (i.e. if the proxy represents a relevant share of the impacts of the product).

- **Molecular Structure Models:** these models are applied to chemicals. They calculate environmental impacts comparing the chemical based on the assumption that similar molecular structures imply similar life cycle impacts, due to similarities in the chemical pathways used to create that structure.

While the first two approaches have limitations, they directly utilise information from the specific process under assessment, aligning with the definition of foreground. By contrast, the last two approaches rely entirely on data for a different chemical or material, and therefore should be considered as a last resort.

5.3.2 Background system

To model the entire life cycle of a chemical or material, the assessor must also select appropriate data on the background system. Figure 20 previously mentioned above shows an innovative process which involves reagents that are chemicals available on the market from established processes. Hence, these reagents have data associated with them, which can be used in modelling their production. Since primary data might not be available to model the background system, there are some strategies to deal with the modelling of the background according to the processes needed, and to the available information.

Background datasets can be found in various LCA databases, but availability may be limited. A fundamental source is the Global LCA Data Access network (GLAD) (UNEP, 2024) which is part of the Life Cycle Initiative hosted by the United Nations Environmental Programme (UNEP), and which acts as a centralised search platform for datasets existing in different LCA databases.

However, some of these procedures, such as the **use of proxy datasets (i.e. a dataset of chemicals that are assumed to be similar to those comprising the target chemicals) and the molecular Structure Based Models (SBM),** may be considered as a viable option only for the modelling of auxiliary chemicals in the life cycle, since such models can be too inaccurate to represent the chemical under assessment. Proxy datasets (method 6 in Parvatker and Eckelman, 2019) rely on assuming strong life cycle similarities between chemicals. If verifiable, this allows using the data from the proxy to build a basic model for the assessed chemical (method 4 in Parvatker and Eckelman, 2019). However, unverified assumptions can introduce significant biases.

Regarding the SBMs, they should be used with caution, since the assumption that the life cycle impacts of a chemical can be inferred by its structure is not always valid. Therefore, Figure 21 can be also used as a guide in the decision of strategies for the filling gaps in the background.

Wernet, Hellweg and Hungerbühler, 2012 proposed an efficient approach for rapidly screening complex mixtures. They employed a shortcut method (SBM) to estimate the impact of minor chemicals, followed by a switch to more accurate proxy data if their estimated impact exceeded a predefined threshold of the overall mixture.

5.3.3 End-of-Life

To model the end-of-life of chemicals, information is needed on the disposal scenario(s) of the product in which the chemical/material is included. It is thus important to understand how the related waste flow is managed, together with the associated disposal method(s). For example, consumer products may be disposed of as a municipal solid waste, while ingredients used in a rinse-off cosmetic product are disposed of through wastewater.

The most relevant sources of information on the topic are statistics on waste management. Since waste management is carried out in a different manner in each EU Member State, the most appropriate scenario is the often that of the average European scenario because Europe (as a whole) is most likely the reference market for a chemical or material.

In LCA, there are several approaches to allocating impacts from waste management, when a recycling process is in place among two life cycles. The suggested approach in the **PEF method is the so-called Circular Footprint Formula (CFF), which allows the assessor to allocate burdens and credits for recycling (and energy recovery)** considering differences in quality between the virgin and the recycled material, as well as the demand-offer of the specific market and the effect of substitution of virgin materials (or energy) (Zampori & Pant, 2019).

The coefficients used in the CFF are constantly updated. However, they are available solely for a limited number of materials, mostly consisting of packaging materials. It is suggested to be cautious in developing *ad hoc* factors for specific cases without strong evidence; furthermore, where there are doubts, it is recommended to conservatively assume that no recycling is taking place.

For additional guidance in the interpretation and application of the CFF, see Damiani *et al.*, 2022.

5.4 Life Cycle Impact Assessment (LCIA)

The SSbD framework recommends the use of the Environmental Footprint (EF) method. Hence, for convenience and coherence with the method, the use of datasets which utilise the same format as the EF should be favoured, or those for which an adapted version of the LCIA method already exists. In simplified LCA, a narrowed down but well justified set of the impact categories might be considered to identify hot-spots directly linked to the goal of the innovation.

The complete set of impact categories considered in the EF is the most accurate way to consider trade-offs along the assessed impacts and to proceed with the results interpretation (See section 5.5).

5.5 Interpretation of results and links to the (re)design

The interpretation of results should be performed to understand:

- The processes, resources, or emissions with the highest contribution; and
- The quality of the model and the data used for the goal of the study.

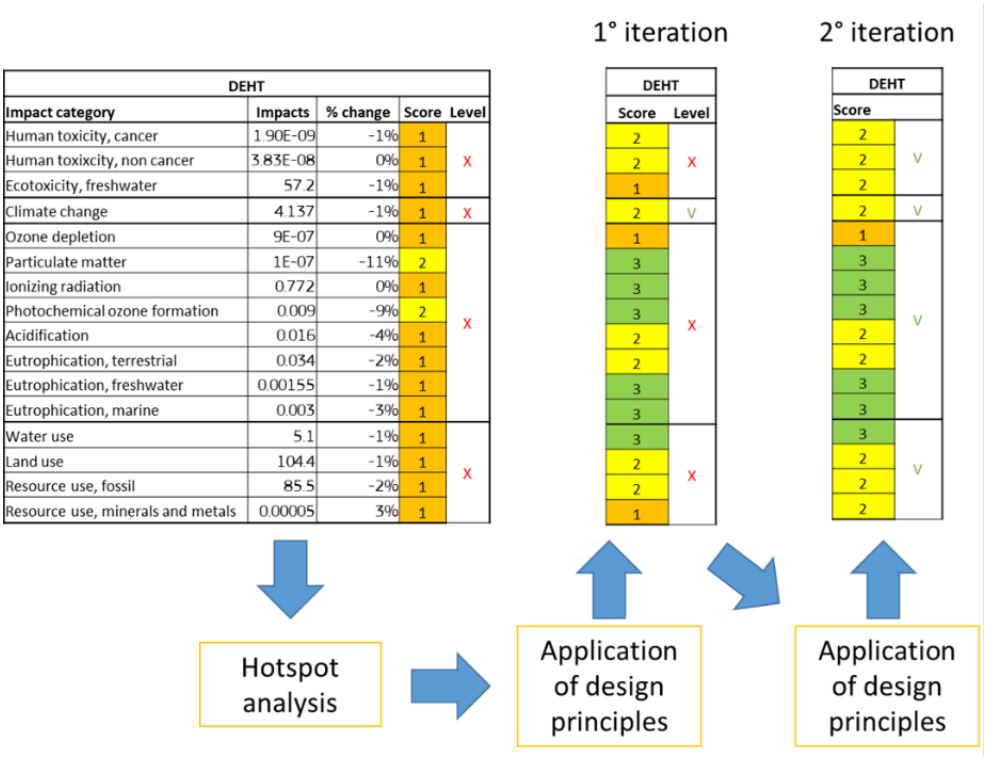
A detailed procedure for the identification of hotspots is described in Section 6 of the PEF methodology (Zampori & Pant, 2019). This allows the identification of the most relevant life cycle stages, processes, and elementary flows. As intended in the original PEF, this is performed to check the robustness of the LCA model, and also to ensure that important processes are modelled appropriately.

In the SSbD context, the **hotspot analysis** is key for the tiered and iterative LCA in the SSbD context:

1) To perform the LCI, through primary data collection or more refined gap filling strategies to reduce uncertainties and to improve the quality of the decision making; and
2) To prioritise the (re)design of aspects along the life cycle of the chemical/material that contribute the most to the LCIA.

Caldeira *et al.*, 2023 illustrates the improvement of the environmental performance of a chemical/material along the innovation process through the iterative approach of the entire SSbD framework (Figure 22).

Figure 22. 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



Source: Caldeira et al., 2023.

5.6 FAQs for the implementation of Step 4

What is meant by the terms "reference" and "benchmark"?

The benchmark represents the basis for comparison for the products with the same function. This is required by ISO 14040 and 14044 and by the PEF methodology (ISO, 2006, 2018; Zampori & Pant, 2019). The representative product is the average product for the definition of the benchmark. The reference chemicals and application can be used as a reference for the innovation process, keeping in mind that the two systems have to be compared based on the functionality. Further explanation is provided in Section 5.2.4.

The suppliers do not want to provide data. How can I deal with this?

In principle, there are databases that fill in any data gaps in LCA. If not, literature reviews can be performed to gather data. The last choice is to use proxies, which are processes of other chemical/material which are similar to the one under assessment for selected reasons. However, the LCA for chemicals/materials requires higher quality data regarding upstream processes. Whenever possible, communication with suppliers is the best choice. This can be mutually beneficial. If this is not possible, sensitivity analyses are crucial to identify the possible parameters and aspects that affect the results the most.

Should I follow the Product Environmental Footprint (PEF) methodology?

The Product Environmental Footprint (PEF) is the suggested methodology by the EC to perform the LCA (European Commission, 2021a). The PEF builds on existing approaches and international standards. The rules provided in the PEF method enable practitioners to conduct PEF studies that are more reproducible, comparable, and verifiable, compared to existing alternative approaches. Nevertheless, it might be challenging to perform such a study at the early stages of the development of a chemical/material. Hence, a simplified version of the PEF study with the increasing complexity and completeness of the modelling can be performed, refining the data and the modelling progressively along the innovation, following the increasing knowledge about the chemical/material. Further information is provided in Section 5.2 of the Methodological guidance.

Is it possible to perform a carbon footprint instead of assessing all the impact categories?

The carbon footprint quantifies the greenhouse gases emissions of a product along its entire life cycle. In the context of the SSbD framework, the carbon footprint should be assessed for the chemical/material under assessment. However, the quantification of the carbon footprint is narrowed down to only one impact category (i.e., climate change) with the consequent incomplete assessment. The SSbD assessment, and more precisely Step 4 of the SSbD, aims to provide a holistic assessment of the environmental impact which cannot consider solely climate change. In addition, the effort dedicated to the data collection and generation is needed, regardless of the number of impact categories considered. Nevertheless, discussions and interpretations for all the impact categories need to be made to identify hotspots and the quality of the results.

What are the Planetary Boundaries (PBs)?

The Planetary Boundaries is a type of framework which aims to assess the limit within which humanity and ecosystems can develop and thrive for generations. There are currently nine planetary boundaries assessed, of which six are currently transgressed. Crossing boundaries increases the risk of large-scale abrupt or irreversible environmental changes that can undermine human development. More information and updates on the topic can be found at the Stockholm Resilience Centre website (Diamond et al., 2015; Stockholm Resilience Centre, 2024).

How are the different impact categories of the Environmental Footprint method linked to the Planetary Boundaries (PBs)?

The environmental impacts measured with LCA have been linked to the Planetary Boundaries through a cause-effect link, where possible. This procedure allows one to calculate a threshold for the safe zone of each impact category. The details of this procedure can be read in detail in Sala *et al.*, 2020.

How can LCA results be aggregated to obtain a single weighted SSbD score?

Once the LCA results are obtained, the comparative assessment requires that the reference is assigned the score of "1" for each impact category. According to the scoring system for Step 4 (shown in Table 50 of the case study, (Caldeira et al., 2023)), all the alternatives are compared to the reference. Once all the scores are assigned, the impact categories can be aggregated to aid the decision making and the hotspots identification. Caldeira et al., 2022a propose an aggregation at the level of four separate groups, to determine the level for each impact category group:

- Toxicity: Human toxicity - cancer, human toxicity – non cancer, and Ecotoxicity - freshwater
- Climate change
- Pollution: aggregating Ozone depletion, particulate matter, Ionizing radiation – Human health, Photochemical ozone formation – human health, Acidification, Eutrophication – terrestrial, Eutrophication – freshwater, and Eutrophication – marine
- Resources: water use, land use, resource use – fossil, and resource use – minerals and metal

6 How to perform a socio-economic assessment within the SSbD framework

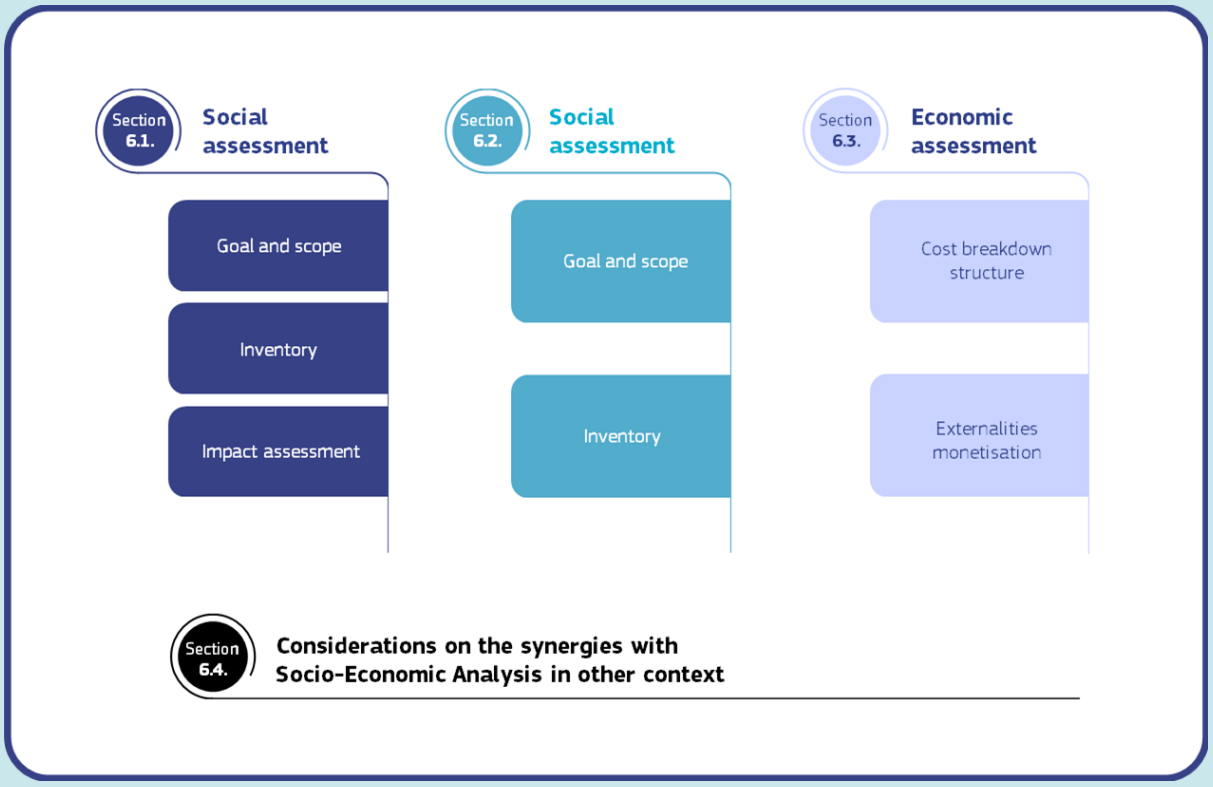
AIM OF THE SECTION:

The socio-economic assessment is an optional step in the SSbD framework, not included in the EC Recommendation, due to the lower methodological maturity of the related disciplines. The figure below illustrates the main elements of the guidance for this optional step. The following approaches are suggested:

- For the **social assessment**: assess social performances and risks along the life cycle using a Reference Scale method.
- For **Critical Raw Materials** (CRMs): flag the presence of CRMs by screening the life cycle inventories.
- For the **economic assessment**: apply monetisation factors to the results of the LCA.

Finally, it highlights the synergies and links with other socio-economic analysis performed at corporate level.

STRUCTURE OF THE SECTION:



Source: Own elaboration

6.1 Social assessment

Social assessments at product level are usually performed by means of Social LCA (S-LCA). The main methodological guidance is the UNEP Guidance (UNEP, 2020), providing a detailed description of all the steps of the methodology; the Handbook for Product Social Impact Assessment (Goedkoop et al., 2020) and the deliverables of the Horizon 2020 project ORIENTING (Grant agreement No 958231) are other references which provide recommendations for companies applying the Life Cycle Sustainability Assessment methodology.

The S-LCA methodology mirrors the Environmental Life Cycle Assessment (LCA) with four key phases: defining goals and scope, inventorying life cycle data, assessing impacts, and interpreting results. However, S-LCA diverges in its focus on stakeholder identification, the selection of impact categories, and evaluation of both negative and positive impacts.

For companies, S-LCA offers a means to pinpoint "hotspots" where social risks are concentrated, supporting supply chain due diligence efforts to address environmental and social impacts proactively. By detecting and mitigating social risks, companies can safeguard their reputation and enhance the social sustainability of their products.

Within the framework of Safe and Sustainable by Design (SSbD), a simplified S-LCA can be employed to uncover potential social risks and opportunities within the supply chain of a chemical or material, and in the evaluation of alternatives. This streamlined approach allows the identification of phases in the supply chain where issues like poor working conditions or threats to local communities may arise. Conversely, it also sheds light on the social benefits that may stem from production activities, such as creating local employment opportunities or contributing to economic development.

This section offers practical guidance on the key steps of the methodology, i.e. the goal and scope (Section 6.1.1), social inventory (Section 0), and the social impact assessment (Section 6.1.3).

6.1.1 Goal and scope

In S-LCA, the goal and scope phase requires the definition of several aspects, i.e.: the intended application of the study, the intended target audience, the reason for conducting the study, the functional unit, the life cycle stages, and processes included in the study, the system boundaries. In an SSbD study, these aspects are addressed in the previous steps of the analysis, particularly in the scoping phase and in Step 4. However, for the social assessment, the goal and scope phase should be complemented by the following tasks:

- **Identify the organisations** involved in the different steps of the product system: in addition to the product system described in Step 4, the organisations involved in the supply chain, their role (e.g. supplier, distributor), location and the level of relationship with the organisation should be specified. While this phase can be time consuming, this can build upon the scoping analysis phase, which includes the identification of key actors in the life cycle.
- **Select potential country-sector combinations** for the steps with unknown organisations, to allow the use of secondary data from S-LCA databases. Scenarios testing different countries can be applied, aligning with the assumptions and scenarios outlined in Step 4 of the framework. (Figure 23).
- **Perform a materiality assessment** to define which are the material/relevant social topics through the life cycle (see Box 3). A “materiality assessment” is a process to define topics that

are important because of their impact on stakeholders/business and/or because they are considered relevant by the target audience who desire to have information on them (Pihkola et al., 2022). Where the materiality assessment has been already addressed within the organisation (as part of e.g. the sustainability reporting directive), the analysis should be adapted considering the specific chemical/material under investigation. The reference list of social topics to be screened is shown in Figure 24.

- Define the **stakeholder categories**, i.e. groups of people affected (positively or negatively) by the product life cycle according to social topics which stem from the materiality assessment. The reference list of stakeholders recommended by UNEP, 2020 is likewise shown in Figure 24. However, additional group or subgroups (e.g. migrant workers) can be added if relevant for the study.

Figure 23. Example of a generic system boundary for the social assessment

Source: Own elaboration

Figure 24. List of stakeholder categories and impact subcategories defined by the S-LCA Guidelines

WORKERS	LOCAL COMMUNITY	VALUE CHAIN ACTORS	CONSUMERS	SOCIETY	CHILDREN
Child labour	Access to material resources	Fair competition	Health and Safety	Contribution to economic development	Education provided in the local community
Forced labour	Access to immaterial resources	Promoting social responsibility	Transparency	Public commitment to sustainability issues	Health issues for children as consumers
Fair salary	Respect of indigenous rights	Supplier relationships	End of life responsibility	Prevention and mitigation of armed conflicts	Children concerns regarding marketing practices
Working hours	Safe and healthy living conditions	Respect of intellectual property rights	Feedback mechanism	Technology development	
Equal opportunities / discrimination	Local employment	Wealth distribution	Consumer privacy	Corruption	
Health and Safety	Delocalization and migration			Ethical treatment of animals	
Social benefits / social security	Cultural heritage			Poverty alleviation	
Freedom of association and collective bargaining	Community engagement				
Employment relationship	Secure living conditions				
Sexual harassment					
Smallholders including farmers					

Source: Own elaboration based on (UNEP, 2020).

Box 3. Performing a materiality assessment

The S-LCA Guidelines recommend choosing relevant social aspects from a set of 40 impact subcategories and six stakeholder categories. To ensure a focused analysis and to avoid bias, a materiality assessment should be conducted, where topics are selected based on their significance to stakeholders and/or the business. Stakeholder engagement, facilitated through dialogue with relevant representatives such as trade unions for workers and NGOs for local communities, informs the materiality assessment process. This assessment also serves as the initial step for sustainability reporting according to the European Sustainability Reporting Standard (ESRS) mandated by the Directive on Corporate Sustainability Reporting (European Commission, 2022b). This directive requires a double materiality assessment, considering both financial and impact materiality, emphasising issues significant for financial reasons or various sustainability aspects.

Four main phases are recommended in order to perform this analysis (Pihkola et al., 2022):

(i) Describing the life cycle of the chemical/material (adapting it from SSbD step 4) and the context of the organisation conducting the assessment;

(ii) Identifying actual and potential sustainability impacts of the chemical/material (identifying relevant topics using as a starting point the list of social impact subcategories recommended by UNEP 2020, Figure 24);

(iii) Assessing the significance of potential impacts based on available information (e.g. via a literature review, feedback from stakeholders, interviews with experts);

(iv) Prioritising the most significant impacts and identifying preliminary improvement options.

Table 5 shows how the materiality assessment was conducted in a case study on technical coat within the EU project ORIENTING. Material topics were identified per life cycle stage and at the level of the overall life cycle. The level of materiality or importance was defined according to a five-point Likert scale. The identification of material social topics was carried out combining two approaches: i) desk review of social aspects highlighted in sector-specific literature and policy papers; ii) participative techniques, to elicit the views and needs of the industrial stakeholders in the ORIENTING consortium.

Table 5. Assigned importance of social topics along the life cycle of technical coat (examples). The scale ranges from 1/grey: not important to 5/darker blue: very important

Social topics	1. Raw materials acquisition and pre-processing	2. Manufacturing	3. Distribution	4. Use	5. End of life
1. Access to material resources	5	5	3	1	1
2. Affordability	3	4	2	4	1
3. Child labour	5	5	1	1	1
4. Community engagement	4	3	1	1	1
5. Contribution to economic development	5	3	3	3	1
6. Corruption	5	5	4	3	1
7. Delocalization and migration	4	4	1	1	1
8. Discrimination and equal opportunities	4	4	1	1	1
9. Health and safety	5	5	5	1	1

Source: Own elaboration Adapted from Pihkola et al., 2022.

6.1.2 Social inventory

The LCI consists of modelling the product system and collecting all the data and information that is needed for conducting the assessment. Data needs and requirements depend on the goal and scope of the study and the specific social topics selected in the goal and scope phase.

For the social assessment, both quantitative and qualitative data can be used for the assessment. Overall, data and information can be classified in these two main groups*:*

- **Primary data** (company or site-specific data): These data describe the behaviour of the organisation(s) and are used to measure the **social performances** of those processes under the direct/indirect control of the company conducting the assessment. The primary data should be collected to reflect company specific behaviour, measured only by referring to specific and real situations, capturing both negative and positive aspects. An example of social performance for the social topic "discrimination and equal opportunities" is whether the organisation has formal policies in place on equal opportunities and what these consist of;
- **Secondary data** (sector or country level data) consist of information from statistics and databases that describe the likelihood that a certain social topic is relevant, and are used for assessing **social risks**, especially in the background processes (i.e. not directly controlled by the organisation performing the study). These types of data can be used for both social risk assessment (or hotspot analysis) and for complementing information on the remote parts of the life cycle in a performance assessment when no direct information or data are available. For example, if it is not possible to know the rate of accidents at work in an upstream phase of the supply chain, it is possible to use country-sector estimates on these aspects from the available databases (see Zanchi *et al.*, 2023).

Both for primary and secondary data, where there is a lack of data, missing parts of data or other limitations, these must be clearly documented, as this will help the interpretation of the results.

A **data quality assessment** must be conducted as part of the inventory phase. During the data quality assessment, the accuracy and robustness of the input data is assessed according to a set of criteria:

- Reliability of the source(s);
- Completeness conformance;
- Temporal conformance (i.e. are the data recent?);
- Geographical conformance (e.g. are the data pertinent to the operations and sites?);
- Further technical conformance (e.g. are the data specific for the sector under investigation?).

Details on the data quality assessment can be found in Zanchi et al., 2023.

The **selection of specific indicators** for the assessment of social risks and performances can be guided by the resources available, e.g.:

- UNEP Methodological Sheets for Subcategories in S-LCA (UNEP, 2021)
- ORIENTING D2.5c Performance indicators for Social LCA (Pihkola et al., 2022)
- Handbook for Product Social Impact Assessment (Goedkoop et al., 2020).
- S-LCA databases (e.g. Product Social Impact Life Cycle Assessment database (PSILCA) Social Hotspot Database (SHDB).

6.1.3 Social impact assessment

The impact assessment phase characterises the magnitude and significance of impacts caused by the product system. Given the complexity of assessing the cause-effect chain that connects a certain

activity to a change in the wellbeing of stakeholders, it is recommended for the S-LCA, in the context of the SSbD, to assess the social performances and social risk along the whole life cycle according to the **Reference Scale Approach** (RSA). In RSA, social performances and risks are evaluated based on pre-defined, specific reference points of expected activity. The approach does not establish a direct link between the activity and long-term impacts but rather estimates the likely magnitude and significance of potential impacts in the assessed product system (UNEP, 2020).
In the context of SSbD, the impact assessment phase facilitates comparing alternatives considering potential risks and issues of concern for the social sustainability.
Both for performance and risk assessment, it is essential to define and use reference scales, i.e. ordinal scales, quantitative (i.e. from 1 to 5) or qualitative (i.e. from Very low to Very high; from ideal performance to non-compliance). These scales should correspond to levels of risk or performance related to known intervals and thresholds.
For the performance assessment, the reference scale developed in ORIENTING is recommended (Pihkola et al., 2022). It consists of a five-levels scoring system, from -2 to +2, applicable to every social topic. Each scale level is described by performance indicators, attributed to each social topic in the scope of the study. Generally, the level +2 corresponds to the ideal performance, while the worst performance (-2) corresponds to non-compliance or no action taken. Detailed description of the reference scales proposed in Orienting is available in Zanchi et al., 2023.

Concerning the **risk assessment**, the PSILCA database provides risk levels for a set of social indicators (Maister et al., 2020) grouped into 25 social subcategories (social topics). The latest version gives 69 indicators, measured in different units, such as single values or percentages, and some of the indicators are qualitative. Risk levels range from "very low risk" to "very high risk" with intermediate levels called low, medium, high and no risk. The level of risk is attributed to the indicator based on the social raw value and the specific reference scale.
An example of reference scale for the indicator “Rate of fatal accidents at workplace” is presented in Table 6. When performing the SSbD case study, the risk levels assigned by PSILCA (from very low to very high) were assigned to points in line with the assessment scheme of the other SSbD steps (Caldeira et al., 2023).

Table 6. Reference scale used to assess the indicator “fatal accidents at work”

Rate of fatal accidents at workplace		
Unit: # per 100k employees		
Indicator value	**Risk level**	**Points assigned**
0 ≤ y < 7.5	Very low risk	4
7.5 ≤ y < 15	Low risk	3
15 ≤ y < 25	Medium risk	2
25 ≤ y < 40	High risk	1
40 ≤ y	Very high risk	0

Source: Caldeira et al., 2023, adapted from the reference scale available in PSILCA.

The **Aggregation** of results allows the results to be combined and then synthesised. This gives an overview understanding of the outcomes of the assessment, facilitating. In principle, aggregation can occur across impact categories, life cycle stages, and stakeholder categories. This process often

involves applying weights to reflect their relative importance. Even when weighting is not explicitly stated, an implicit weighting is assumed, treating all contributing indicators as equally relevant. Given that the aggregation within S-LCA is not well developed, it is recommended to limit the aggregation to within a particular social topic, following the semi-quantitative dual flag approach proposed in ORIENTING 2023 D.2.5. In general, compensation between positive and negative impact within or across different social topics and stakeholder groups should be avoided. For example, a negative performance on child labour by one supply chain actor, should not be compensated in an aggregation score by positive performance on health and safety for the consumer.

6.2 Criticality assessment in the supply chain

The EU definition and methodology defines CRMs as those materials with relatively higher economic importance for the EU economy and with higher supply risks associated to them, due to the increased concentration of supply from countries with weak governance (European Commission, 2017). The limited substitutability of these materials may also increase their criticality, which in turn leads to a risk of supply disruption and can be reflected in higher prices in the market. The EU assessment of CRMs is performed every three years. The list of CRMs identified by the last assessment in 2023 includes 30 raw materials.

In the design of safe and sustainable chemicals, tracing the use of CRMs in the supply chain at company level should be part of a business-risk-mitigation strategy to increase awareness about potential supply chain vulnerabilities. Indeed, when substituting harmful substances with safer and more sustainable alternatives, companies could also consider the criticality of materials used in the supply chain and aim to minimise their reliance on CRMs. In the future, CRMs might become (even) more expensive or scarcer given that they often originate from countries with poor governance. Finally, the CRM analysis allows the consideration of the role of advanced materials, seen as an alternative for CRMs, for companies to use in a possible CRM substitution strategy.

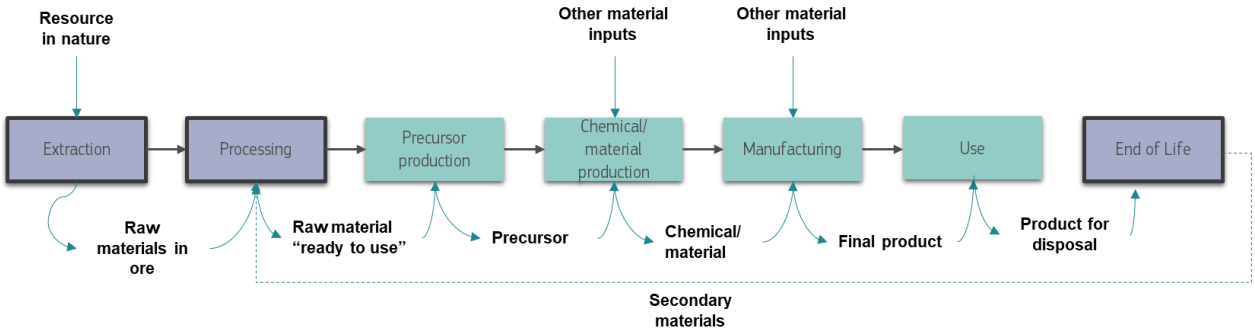
6.2.1 Goal and scope phase

The main objective of this phase is to set the boundaries for the assessment of CRMs in the life cycle of the chemicals/materials considered. Starting from the system boundary developed in Step 4, it is important to identify the steps where input flows of critical raw materials occur, as well as understanding which CRMs could be recovered from the disposal of the final product. Figure 25 highlights the potential raw materials flows in a generic system boundary of a chemical or material.

Once the system boundary is set, the following information should be collected:

- Identification of the main raw materials used as precursors in the production of the chemical/material under consideration via the Bill of Materials (BoM), which gives an overview of the minerals, metals, fossil fuels and natural biomass.
- Investigate what is the origin of these materials, which will help understanding potential issues related to the governance of supplying countries and economic availability.
- Check if this material is critical according to EC list of CRMs (European Commission, 2023).
- Identify the main raw materials present in the life cycle of the final product, considering the potential applications of the chemical/material under investigation. This information can come from Life Cycle Inventories of products that are expected to use the chemicals/materials under investigation.

Figure 25. System boundaries for the analysis of CRMs in the supply chain. The squares with bold outline indicate the most relevant phases for the identification of CRMs



Source: Own elaboration

6.2.2 Inventory phase

For this phase, the inventory data collected to perform the (environmental) LCA can again be utilised (See Section 5.3). Both the inventories of the LCA foreground system and those used for the LCA's background system should be considered (see Section 5.3 for Step 4).

From these inventories, only the input flows of raw materials and the output flows of products (products, co-products, and by-products) and waste are relevant to assess the criticality. The mass of CRMs entering in the product system should be accounted for and compared in an evaluation of alternatives. This information will provide a basis for exploring materials substitution opportunities for considering the potential risk of supply disruption in the life cycle of the chemical/material. The output materials flows, in terms of waste or by-products, should also be checked to understand which are the losses of CRMs and investigate if material recovery would be feasible.

6.3 Economic assessment and evaluation of externalities

In the context of a life cycle sustainability assessment, economic considerations are assessed via the Life Cycle Costing (LCC) methodology. The LCC consists of accounting for all the costs that accrue in the life cycle of a product with reference to one or more participants in the product system (Bianchi et al., 2021). In the context of an SSbD study, the LCC can be used to compare life cycle costs of alternatives, detecting direct and indirect (hidden) cost drivers, or estimating improvements of planned product changes, including process changes within a life cycle or via product/process/component innovations. Moreover, an LCC assessment can support the identification of win-win situations and trade-offs in the life cycle of a product, once it is combined with LCA.
The LCC methodology has been applied using a variety of approaches and three main types can be distinguished (Bianchi et al., 2021):

- Conventional LCC (cLCC), which is the assessment of all costs associated with the life cycle of a product and covered by actors. It usually considers the perspective of the producer only.
- Environmental LCC (eLCC), which extends the conventional LCC including environmental externalities and a comprehensive stakeholder perspective.
- Societal LCC (sLCC), which further extends the environmental LCC by including additional externalities, associated with the life cycle of a product, i.e. societal externalities that are not borne by any of the lifecycle actors during the relevant time period.

In the context of an SSbD study, the environmental LCC (eLCC) is the most appropriate methodology and can be applied in a modular and incremental approach, starting from a basic conventional LCC (cLCC), and then adding the perspectives of other stakeholders including the evaluation of environmental externalities.

The steps to undertake for the economic analysis are the following:

- Firstly, develop a **cost breakdown structure**, to identify, define and organise all cost elements to be considered. These costs elements are organised according to the phase of the product life cycle, to perceive how costs are distributed along the product life cycle. Here, we can consider the solely perspective of the producer, OR include more stakeholders (e.g. the product user, society). Common types of costs include capital costs, material/utilities costs (gas, electricity, water, etc.), personnel costs, transport cost, etc. Detailed guidance on the cost breakdown structure can be found in (Pihkola et al., 2022).
- **Monetisation of externalities:** Externalities can be defined as "consequence of an activity that affects interested parties other than the organisation undertaking the activity, for which the organisation is neither compensated nor penalised through markets or regulatory mechanisms" (ISO, 2019). This step allows converting measures of societal and biophysical impacts calculated in Step 4 into monetary units. Via assigning a monetary valuation for different environmental impact categories this allows an aggregation into one single value (based on the currency chosen) from different environmental results. This requires applying a set of monetary valuation coefficient (MVC) to life cycle impact assessment methods. Note that such valuation methods are sometimes controversial, with a lack of acceptance among some stakeholders. Given the large variability of the MVC sets available in literature and in policy documents, the JRC performed a review and proposed a set of MVC to be applied in the context of the Ecodesign of energy-related products (Gama Caladas et al., 2024), (Table 7). For some impact categories, however, it was not possible to give a recommendation on the related MVC.

Table 7. Preliminary set of monetary valuation coefficients as proposed in the context of Ecodesign

	Impact category	Unit of measure	Value
1	Climate change, total	$€_{2019}$/kg CO_2 eq.	$1.00x10^{-1}$
2	Ozone depletion	$€_{2019}$/kg CFC-11 eq.	$5.55x10^{+1}$
3	Human toxicity, cancer	$€_{2019}$/CTUh	$1.66x10^{+5}$
4	Human toxicity, non-cancer	$€_{2019}$/CTUh	$9.19x10^{+5}$
5	Particulate matter	$€_{2019}$/disease incidence	$7.28x10^{+5}$
6	Ionising radiation, human health	$€_{2019}$/kBq U_{235} eq.	-
7	Photochemical ozone formation, human health	$€_{2019}$/kg NMVOC eq.	$1.20x10^{0}$
8	Acidification	$€_{2019}$/mol H^+ eq.	$3.50x10^{-1}$
9	Eutrophication, terrestrial	$€_{2019}$/mol N eq.	-
10	Eutrophication, freshwater	$€_{2019}$/kg P eq.	$1.95x10^{0}$
11	Eutrophication, marine	$€_{2019}$/kg N eq.	$3.27x10^{0}$
12	Ecotoxicity, freshwater	$€_{2019}$/CTUe	$3.89x10^{-5}$
13	Land use	$€_{2019}$/pt	$1.78x10^{-4}$
14	Water use	$€_{2019}$/m^3 water eq. of deprived water	$5.08x10^{-3}$
15	Resource use, minerals, and metals	$€_{2019}$/kg Sb eq.	-
16	Resource use, fossils	$€_{2019}$/MJ	-

Source: Gama Caldas et al. 2024

6.4 Concluding remarks on synergies with other socio-economic analysis

The identification of social performance and risks is becoming an increasingly relevant need, especially for companies operating in global value chains. This is also increasingly required by consumers, business-to-business relationships, and legislation both at national and EU level.

Companies operating in the chemical sector may face the need to perform socio-economic analysis in the context of authorisation processes for new substances.

Existing and upcoming regulatory requirements as well as market demand for greener and ethical supply chains, will increasingly push companies towards an increased effort in terms of data collection and engagement with actors in the value chain. In this context, synergies can be identified with this optional Step of the SSbD, given that some tasks performed by companies or data collected for other purposes can also be used for the socio-economic assessment of the SSbD. Table 8 summarises the main common elements between the SSbD and the most relevant related socio-economic assessment performed under the EU legislation (present or upcoming).

Table 8. Envisaged synergies between the socio-economic assessment in SSbD and other socio-economic analysis

Policy/Document	**Level of assessment**	**Aim**	**Envisaged synergies with socio-economic assessment in SSbD**
Corporate Sustainability Reporting Directive (CSRD) (European Commission, 2022b)	Corporate	Establishes rules concerning the social and environmental information that companies have to report, through the European Sustainability Reporting Standards (ESRS).	- Materiality assessment - Assessment of performance through the Reference Scale Approach
Corporate sustainability due diligence directive proposal (CSDDD) (COM/2022/71 final – undergoing co-decision procedure; to be adopted in 2024) (European Commission, 2022c)	Corporate	Requires companies operating within the European Union to conduct due diligence throughout their supply chains to identify, prevent, mitigate, and account for adverse impacts on human rights, the environment, and governance issues.	- Modelling of the supply chain - Identification of social risks - Engagement with business relationships in the value chain.
Socio-Economic Analysis within the ECHA authorisation process under REACH regulation (ECHA, 2011b)	Substance	Assess the socio-economic impacts of the continued use of a substance subject to authorization, or in the assessment of alternatives	- Identification of social impacts - Data collection on e.g. working conditions - Definition of scenarios for application/use of the chemical/material - Economic analysis and cost breakdown structure

Source: Own elaboration

6.5 FAQs on the socio-economic assessment

How can I deal with qualitative data in the socio-economic assessment?

Qualitative data describes the attributes or properties of an object or an activity. For instance, the performance of an organisation concerning workers' health and safety can be assessed describing the extent to which the company puts in place preventive measures (among other indicators). Descriptions of properties or performances can be categorised into classes that may be assigned numeric values and be included in a scoring system in line with the other steps of the SSbD framework.

What is the difference between foreground and background process in the socio-economic assessment?

In S-LCA, the foreground system corresponds largely to the terminology as used in LCA. To this end, it includes all the processes that can be directly studied, and for which specific data can be collected. Therefore, this means activities carried out by the company performing the assessment and eventually direct suppliers or users for which it is possible to collect the data. The background system includes further upstream or downstream processes in the product system, for which generic data from databases can be used.

How can I proceed if I do not know have enough information on the upstream phases of the supply chain?

If the origin of precursors and raw materials used in the production of a chemical/material is unknown, assumptions can be made using statistics on the main countries supplying certain materials or chemicals used as precursors, as done in the SSbD case study on plasticiser (Caldeira et al. 2023). If several countries are likely to be involved in the supply of a certain chemical/material, different scenarios can be tested.

Can I perform the socio-economic analysis if I do not have a licence for a commercial S-LCA database?

The S-LCA databases can facilitate the analysis as they provide reference scales and social risks levels for a broad set of country-sector combinations. However, the analysis can also be performed using open-source data bases like the International Labour Organization (which collects data on many social aspects, like child labour, fair salary, accident at work, etc.).

What is the difference between corporate sustainability reporting and socio-economic assessment in the context of SSbD?

Corporate sustainability reporting is a legal obligation for companies above certain size under the Corporate Sustainability Reporting Directive (EU 2022). The European Sustainability Reporting Standards (ESRS) provide guidance for reporting under this Directive. In this context, the reporting is performed at corporate level, with the aim of helping investors, civil society organisations, consumers, and other stakeholders to evaluate the sustainability performance of companies. In the context of the SSbD framework, the socio-economic assessment is an exploratory phase which is not part of it, as such (European Commission 2022). The socio-economic analysis could support research and innovation in the assessment of alternatives for substitution of a substance, towards the identification of safer and more sustainable solutions. As far as possible, the socio-economic analysis should be conducted at the level of substance/product, detecting social risks and benefits along its potential supply chain.

What is the link between socio-economic assessment and SDGs?

The S-LCA methodology can support the monitoring of SDG 12 on Responsible Consumption and Production and also has relevant connections with ten other SDGs: (1) No Poverty, (2) Zero Hunger, (3) Good Health and Well-Being,

(4) Quality Education, (5) Gender Equality, (6) Clean Water and Sanitation, (8) Decent Work and Economic Growth, (10) Reduced Inequalities, (16) Peace, Justice and Strong Institutions, and (17) Partnerships for the Goals. S-LCA can also support Goal 8 of the 2030 Agenda, which calls for the promotion of long-lasting, inclusive, and sustainable economic growth, full and productive employment, and decent work.

References

Bianchi, M., Bachmann, T. M., Kamp, J. van der, Riemer, M., Riva, F., Préat, N., & Taelman, S. E. (2021). *Orienting D1.3 - Critical evaluation of economic approaches* (Issue January). https://doi.org/10.13140/RG.2.2.26482.22721

Buchner, G. A., Stepputat, K. J., Zimmermann, A. W., & Schomäcker, R. (2019). Specifying Technology Readiness Levels for the Chemical Industry. *Industrial and Engineering Chemistry Research*, *58*(17), 6957–6969. https://doi.org/10.1021/acs.iecr.8b05693

Caldeira, C., Farcal, R., Garmendia Aguirre, I., Mancini, L., Tosches, D., Amelio, A., Rasmussen, K., Rauscher, H., Riego Sintes, J., & Sala, S. (2022). Safe and Sustainable chemicals and materials by Design: Framework for the definition of criteria and evaluation procedure for chemicals and materials. *EUR 31100 EN, Publications Office of the European Union, Luxembourg, 2022, ISBN 978-92-76- 53264-4, Doi:10.2760/487955, JRC128591*. https://publications.jrc.ec.europa.eu/repository/handle/JRC128591

Caldeira, C., Farcal, R., Moretti, C., Mancini, L., Rauscher, H., Rasmussen, K., Riego, J., & Sala, S. (2022). Safe and Sustainable chemicals by design chemicals and materials: Review of safety and sustainability dimensions, aspects, methods, indicators, and tools. *EUR 30991 EN, Publications Office of the European Union, Luxembourg, 2022, ISBN 978-92-76-47560-6, Doi:10.2760/879069, JRC127109*, *March*, 1–185. https://publications.jrc.ec.europa.eu/repository/handle/JRC127109

Caldeira, C., Garmendia Aguirre, I., Tosches, D., Mancini, L., Abbate, E., Farcal, L., Lipsa, D., Rasmussen, K., Rauscher, H., Riego Sintes, J., & Sala, S. (2023). Safe and Sustainable by Design chemicals and materials - Application of the SSbD framework to case studies. *Publications Office of the European Union, Luxembourg, 2023, JRC131878*. https://publications.jrc.ec.europa.eu/repository/handle/JRC131878

CEFIC. (2024). *ECEL 3.0 – INTEGRATED RISK MANAGEMENT MEASURE LIBRARY [Last access: May 2024]*. https://cefic-lri.org/toolbox/ecel-3-0-integrated-risk-management-measure-library/

Charnes, A., Cooper, W., & Rhodes, E. (1978). Measuring the efficiency of decision making units. *European Journal of Operational Research*, *2(6):429-444*. https://doi.org/10.1016/0377-2217(78)90138-8

Charnes, A., & Cooper, W. W. (1957). Management Models and Industrial Applications of Linear Programming. *Management Science*, *4(1):38-91*. https://doi.org/https://doi.org/10.1287/mnsc.4.1.38

Damiani, M., Tosches, D., Zamagni, A., Zampori, L., & Ardente, F. (2022). Advancing on comparability aspects for Product and Organisation Environmental Footprint. *EUR 31308 EN, Publications Office of the European Union, Luxembourg, 2022, Doi:10.2760/47763, JRC130715*. https://doi.org/10.2760/47763

Danish EPA. (2024). *Danish (Q)SAR Database [Last access: May 2024]*. https://qsar.food.dtu.dk/

Diamond, M. L., de Wit, C. A., Molander, S., Scheringer, M., Backhaus, T., Lohmann, R., Arvidsson, R., Bergman, Å., Hauschild, M., Holoubek, I., Persson, L., Suzuki, N., Vighi, M., & Zetzsch, C. (2015). Exploring the planetary boundary for chemical pollution. *Environment International*, *78*, 8–15. https://doi.org/10.1016/j.envint.2015.02.001

EC-JRC. (2024). *QSAR Model database [Last access: May 2024]*. https://jeodpp.jrc.ec.europa.eu/ftp/jrc-opendata/EURL-ECVAM/datasets/QSARDB/LATEST/qsardb.html

ECHA. (2011). *Guidance on the preparation of socio-economic analysis as part of an application for authorisation - version 1*. https://echa.europa.eu/it/view-article/-/journal_content/title/guidance-on-socio-economic-analysis-authorisation

ECHA. (2012). *Guidance on information requirements and chemical safety assessment Chapter R . 13 : Risk management measures and operational conditions October 2012 Version 1.2*. 1–30.

ECHA. (2015). *Guidance on information requirements and chemical safety assessment - Chapter R.12 : use description, version 3.0*. https://echa.europa.eu/documents/10162/17224/information_requirements_r12_en.pdf

ECHA. (2024). *Use maps libraries, ECHA [last access: May 2024]*. https://echa.europa.eu/csr-es-roadmap/use-maps/use-maps-library

EPA. (2024). *EPI Suite™-Estimation Program Interface [Last access: May 2024]*. https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

European Commission. (2017). *COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS on the 2017 list of Critical Raw Materials for the EU*. *COM(2017)*(490), 8. https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:52017DC0490&from=EN

European Commission. (2019). *COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE EUROPEAN COUNCIL, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS The European Green Dea*. *COM(2019)*(640). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52019DC0640

European Commission. (2020). *Communication from the Commission to the European Parliament, the Council, the European Economic and Social Committee and the Committee of the Regions. Chemicals Strategy for Sustainability Towards a Toxic-Free Environment*. *COM(2020)*(667). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52019DC0640

European Commission. (2021a). *COMMISSION RECOMMENDATION of 16.12.2021 on the use of the Environmental Footprint methods to measure and communicate the life cycle environmental performance of products and organisations*. *C(2021)*(9332). https://environment.ec.europa.eu/system/files/2021-12/Commission Recommendation on the use of the Environmental Footprint methods_0.pdf

European Commission. (2021b). *COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS Pathway to a Healthy Planet for All EU Action Plan: "Towards Zero Pollution for Air, Water and Soil." COM(2021)*(400). https://eur-lex.europa.eu/resource.html?uri=cellar:a1c34a56-b314-11eb-8aca-01aa75ed71a1.0001.02/DOC_1&format=PDF

European Commission. (2022a). COMMISSION RECOMMENDATION (EU) 2022/2510 of 8 December 2022 establishing a European assessment framework for "safe and sustainable by design" chemicals and materials. *Official Journal of the European Union*, *325/179*(July 2020). https://doi.org/10.2760/879069

European Commission. (2022b). DIRECTIVE (EU) 2022/2464 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 14 December 2022 amending Regulation (EU) No 537/2014, Directive 2004/109/EC, Directive 2006/43/EC and Directive 2013/34/EU, as regards corporate sustainability reporting. *Official Journal of the European Union*, *L 322/15*. https://eur-lex.europa.eu/eli/dir/2022/2464/oj

European Commission. (2022c). Proposal for a Directive of the European Parliament and of the Council on Corporate Sustainability Due Diligence and amending Directive (EU) 2019/1937. *Official Journal of the European Union*, *COM(2022)*(71). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A52022PC0071

European Commission. (2022d). *Proposal for REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL establishing a framework for setting ecodesign requirements for sustainable products and repealing Directive 2009/125/EC*. *COM(2022)*(142). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52022PC0142

European Commission. (2023). *Proposal for a REGULATION OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL establishing a framework for ensuring a secure and sustainable supply of critical raw materials and amending Regulations (EU) 168/2013, (EU) 2018/858, 2018/1724 and (EU) 2019/1020*. *COM(2023)*(160). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:52023PC0160

European Commission. (2024). *European Platform on LCA | EPLCA [Last access: May 2024]*. https://eplca.jrc.ec.europa.eu/

European Commission Directorate-General for Research and Innovation. (2021). Mapping study for the development of Sustainable-by-Design criteria. *Amodio, A., Malyska, A., Markouli, C., Soraya, S., Sanfelix, J., Van Humbeeck, T. . Publications Office*. https://doi.org/10.2777/109081

European Parliament and the Council. (2006). Regulation(EC) No1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/. *Official Journal of the European Communities*, *L 396*, *30.12.2006*, pp. *1–849,*. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A02006R1907-20140410

European Parliament and the Council. (2008). REGULATION (EC) No 1272/2008 OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC). *Official Journal of the European Communities L 353, 31.12.2008, p. 1–1355*, 261–295. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=celex%3A32008R1272

European Parliament and the Council. (2010). DIRECTIVE 2010/75/EU OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 24 November 2010 on industrial emissions (integrated pollution prevention and control) (Recast). *Offical Journal of the European Union L 334, 17.12.2010, p. 17–119*. https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX%3A32010L0075

Gama Caladas, M., Spiliotopoulos, C., Alfieri, F., Eynard, U., Zampori, L., Blegini, G. A., Mancini, L., Methieux, F., & Ardente, F. (2024). *Review of the MEErP - Methodology for Ecodesign of Energy-related Products*. https://doi.org/10.2760/24524

Goedkoop, M. J., de Beer, I. ., Harmens, R., Saling, P., Morris, D., Florea, A., Anne Laure, H., Indrane, D., Visser, D., Morao, A., Elizabeth Musoke-Flores;, Alvarado, C., Rawat, I., Schenker, U., Head, M., Collotta, M., Andro, T., Viot, J.-F., & Whatelet, A. (2020). *Roundtable for Product Social Impact Assessment*. 1–88. https://www.social-value-initiative.org/wp-content/uploads/2021/04/20-01-Handbook2020.pdf

Goguen, J. A. (1973). L. A. Zadeh. Fuzzy sets. Information and control, vol. 8 (1965), pp. 338–353. - L. A. Zadeh. Similarity relations and fuzzy orderings. Information sciences, vol. 3 (1971), pp. 177–200. *Journal of Symbolic Logic*, *38*(4), 656–657. https://doi.org/10.2307/2272014

GOV.UK. (2024). *Guidance Non-disclosure agreements (Last access: May 2024)*. https://www.gov.uk/government/publications/non-disclosure-agreements

Hwang, C. L., & Yoon, K. (1981). *Multiple Attribute Decision Making: Methods and Applications—A State-of-the-Art Survey*. https://link.springer.com/book/10.1007/978-3-642-48318-9

Ishizaka, A., & Labib, A. (2009). Analytic hierarchy process and expert choice: benefits and limitations.

OR Insight, *22*, 201–220. https://link.springer.com/article/10.1057/ori.2009.10

ISO. (2006). ISO 14040:2006 Environmental management — Life cycle assessment — Principles and framework. *International Organization for Standardization, Geneva, Switzerland.*

ISO. (2018). ISO 14044:2006+A1:2018 Environmental management - Life cycle assessment - Requirements and guidelines. *International Organization for Standardization, Geneva, Switzerland.*

ISO. (2019). ISO 14007:2019 Environmental management - Guidelines for determining environmental costs and benefits. *International Organization for Standardization, Geneva, Switzerland.*

ISO. (2020). ISO 14044:2006+A2:2020 Environmental management — Life cycle assessment — Requirements and guidelines. *International Organization for Standardization, Geneva, Switzerland.*

Laso, J., Cristóbal, J., Margallo, M., Aldaco, R., & Vázquez-Rowe, I. (2022). Chapter 8 - The combined use of life cycle assessment and data envelopment analysis to analyse the environmental efficiency of multi-unit systems. In C. Teodosiu, S. Fiore, & A. Hospido (Eds.), *Assessing Progress Towards Sustainability* (pp. 137–160). Elsevier. https://doi.org/https://doi.org/10.1016/B978-0-323-85851-9.00008-0

Maister, K., Di Noi, C., Ciroth, A., & Srocka, M. (2020). PSILCA v.3. *PSILCA Documentation*.

Munier, N., & Hontoria, E. (2021). Uses and Limitations of the AHP Method: A Non-Mathematical and Rational Analysis. In *Management for Professionals* (Vol. 1, Issue 2). https://link.springer.com/book/10.1007/978-3-030-60392-2

OECD. (2024). *QSAR Toolbox [Last access: May 2024]*. https://qsartoolbox.org/

Parvatker, A. G., & Eckelman, M. J. (2019). Comparative Evaluation of Chemical Life Cycle Inventory Generation Methods and Implications for Life Cycle Assessment Results. *ACS Sustainable Chemistry and Engineering*, *7*(1), 350–367. https://doi.org/10.1021/acssuschemeng.8b03656

Piccinno, F., Hischier, R., Seeger, S., & Som, C. (2016). From laboratory to industrial scale: a scale-up framework for chemical processes in life cycle assessment studies. *Journal of Cleaner Production*, *135*, 1085–1097. https://doi.org/10.1016/j.jclepro.2016.06.164

Pihkola, H., Cordella, M., Katri, B., Horn, R., Zamagni, A., Zanchi, L., Harmens, R., Sonderegger, T., Cadena Martinez, E., Bachmann, T. M., van der Kamp, J., Bianchi, M., Riva, F., Fehrenbach, D., Moraga, G., Hackenhaar, I. C., Sanchez Moreno, L., Isasa, M., Taelmann, S. E., & Kujanpaa, L. (2022). *ORIENTING D2.3 - LCSA methodology to be implemented in WP4 demonstrations*. 1–208. doi: 10.13140/RG.2.2.24300.13445

RIVM. (2024a). *ConsExpo Web [Last access: May 2024]*. https://www.rivm.nl/en/consexpo/consexpoweb

RIVM. (2024b). *ConsExpo Web fact sheet [Last access: May 2024]*. https://www.rivm.nl/en/consexpo/fact-sheets

Saaty, R. W. (1987). The analytic hierarchy process—what it is and how it is used. *Mathematical Modelling*, *9*(3), 161–176. https://doi.org/https://doi.org/10.1016/0270-0255(87)90473-8

Sacchi, R., Terlouw, T., Siala, K., Dirnaichner, A., Bauer, C., Cox, B., Mutel, C., Daioglou, V., & Luderer, G. (2022). PRospective EnvironMental Impact asSEment (premise): A streamlined approach to producing databases for prospective life cycle assessment using integrated assessment models. *Renewable and Sustainable Energy Reviews*, *160*(March), 112311. https://doi.org/10.1016/j.rser.2022.112311

Sala, S., Crenna, E., Secchi, M., & Sanyé-Mengual, E. (2020). Environmental sustainability of European

production and consumption assessed against planetary boundaries. *Journal of Environmental Management*, *269*. https://doi.org/10.1016/j.jenvman.2020.110686

Schlüter, U., Meyer, J., Ahrens, A., Borghi, F., Clerc, F., Delmaar, C., Di Guardo, A., Dudzina, T., Fantke, P., Fransman, W., Hahn, S., Heussen, H., Jung, C., Koivisto, J., Koppisch, D., Paini, A., Savic, N., Spinazzè, A., Zare Jeddi, M., & von Goetz, N. (2022). Exposure modelling in Europe: how to pave the road for the future as part of the European Exposure Science Strategy 2020–2030. *Journal of Exposure Science and Environmental Epidemiology*, *32*(4), 499–512. https://doi.org/10.1038/s41370-022-00455-4

Stockholm Resilience Centre. (2024). *Planetary boundaries [Last access: May 2024]*. https://www.stockholmresilience.org/research/planetary-boundaries.html

Taherdoost, H., & Madanchian, M. (2023). Multi-Criteria Decision Making (MCDM) Methods and Concepts. *Encyclopedia*, *3*(1), 77–87. https://doi.org/10.3390/encyclopedia3010006

Tsoy, N., Steubing, B., van der Giesen, C., & Guinée, J. (2020). Upscaling methods used in ex ante life cycle assessment of emerging technologies: a review. *International Journal of Life Cycle Assessment*, *25*(9), 1680–1692. https://doi.org/10.1007/s11367-020-01796-8

UNEP. (2020). Guidelines for Social Life Cycle Assessment of Products. *Benoît Norris, C., Traverso, M., Neugebauer, S., Ekener, E., Schaubroeck, T., Russo Garrido, S., Berger, M., Valdivia, S., Lehmann, A., Finkbeiner, M., Arcese, G.*, *United Nations Environment Programme (UNEP)*. https://wedocs.unep.org/handle/20.500.11822/34554;jsessionid=4FC923C0EAB1589CED199ED77ADA5DA0

UNEP. (2021). Methodological Sheets for Subcategories in Social Life Cycle Assessment (S-LCA) 2021. *Traverso, M. Valdivia, S. Luthin, A. Roche, L. Arcese, G. Neugebauer, S. Petti, L. D'Eusanio, M. Tragnone, B.M. Mankaa, R. Hanafi, J. Benoît Norris, C. Zamagni, A.*, *United Nations Environment Programme (UNEP)*.

UNEP. (2024). *Global LCA Data Access network [Last access: May 2024]*. https://www.globallcadataaccess.org/

Wernet, G., Hellweg, S., & Hungerbühler, K. (2012). A tiered approach to estimate inventory data and impacts of chemical products and mixtures. *International Journal of Life Cycle Assessment*, *17*(6), 720–728. https://doi.org/10.1007/s11367-012-0404-0

Zampori, L., & Pant, R. (2019). Suggestions for updating the Product Environmental Footprint (PEF) method. In *Eur 29682 En*. https://doi.org/10.2760/424613

Zanchi, L., Zamagni, A., Pillay, S., Mangana, D., Harmens, R., Pihkola, H., Sonderegger, T., Martinez, E. C., Saling, P., & Isasa, M. (2024). *ORIENTING D2.5 - Specifications of social indicators for LCSA (forthcoming)*.

List of abbreviations and definitions

CLP	Classification, Labelling and Packaging
CRM	Critical Raw Materials
CSR	Chemical Safety Report
CSS	Chemicals Strategy for Sustainability
DEA	Data Envelopment Analysis
DG ENV	Directorate General – Environment
DG RTD	Directorate General - Research and Innovation
EC	European Commission
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
ECHA	European Chemicals Agency
ENES	Exchange Network on Exposure Scenarios
EPA	Environmental Protection Agency
ERC	Environmental Release Category
ES	Exposure scenarios
EU	European Union
FAQ	Frequently asked question
FU	Functional Unit
ISES	International Society of Exposure Science
ISO	International Organization for Standardization
IUPAC	International Union of Pure and Applied Chemistry
JRC	Joint Research Centre
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
MCDM	Multi-Criteria Decision Making
MODM	Multi-Objective Decision Making
NAMs	New Approach Methodologies
NDA	Non Disclosure Agreement
OECD	Organisation for Economic Co-operation and Development
PC	Product category
PEF	Product Environmental Footprint
PROC	Process category
PUC	Product Use Categories
QSAR	Quantitative Structure–Activity Relationship
R&I	Research and Innovation
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDG	Sustainable Development Goal
SDS	Safety Data Sheet
SMILES	Simplified Molecular Input Line Entry System
SSbD	Safe and Sustainable by Design
SU	Sector of use
SVHC	Substance of Very High Concern
TF	Descriptor list for technical functions
TOPSIS	Technique for Order Preference by Similarity to Ideal Solutions
TRA	Targeted Risk Assessment
TRL	Technology Readiness Level

List of boxes

List of figures

List of tables

Annexes

Annex A. Feedback from stakeholders

A.1 Stakeholders' Input to the guidance from the first SSbD testing period

Two voluntary eight-week reporting periods were envisaged, one in May-June 2023 and another in May-September 2024 during which stakeholders are invited to provide feedback and share with the EC their experience. During the first testing period, all interested parties – industry, academia, research and technology organisations, European Union Member States, citizens - were invited to provide feedback, via a reporting template, on their experience with the application of the framework on relevant case studies.

The aim was to obtain insights from users regarding:

- the activities promoting the SSbD framework in R&I programs and policies;
- the SSbD framework's feasibility and applicability by testing it with case studies.

The reporting template guides the users through the SSbD framework and contains several sections that collect essential information regarding the information provider, the chemicals or materials assessed, details regarding the applied SSbD principles, safety and sustainability assessment steps, as well as suggestions for SSbD criteria for chemicals and materials.

A.2 Input to the guidance: Feedback from the Stakeholder Workshops and the 2023 Boot Camp

In addition to the testing periods, two additional opportunities have been offered to stakeholders for providing feedback on the application of the SSbD framework: four SSbD Stakeholder Workshops to date, and the October 2023 SSbD Boot Camp.

Three stakeholder workshops took place while the framework was being developed to discuss and design the SSbD framework. The fourth SSbD Stakeholder workshop, held in Brussels on 4th - 5th December 2023 and co-organised by the JRC and Directorate Generals RTD and ENV, focused on the outcomes of the first reporting period of the SSbD framework, the lessons learnt and the ways forward. The participants physically present at the workshop had the opportunity to discuss specific topics identified among the feedback of the first testing period with the JRC and the other DGs.

Furthermore, the SSbD Boot Camp, was held at JRC-Ispra from 25th to 27th October 2023. It was organised by the JRC in conjunction with the PARC project[3], and had the following aims: to provide fundamental insights into SSbD thinking, to learn about the SSbD framework from experts in the field, and to share knowledge and experience.

[3] Partnership for the Assessment of Risks from Chemicals | Parc (eu-parc.eu)

Annex B. Scoping analysis: guiding questions to define the SSbD system

The present Annex complements the information provided in Section 2 to define the SSbD system. The questions shown in Table B.1 and Table B.2 can be used to guide the definition of the SSbD system under study and to collect some information useful for the SSbD assessment. The list of questions neither exhaustive nor compulsory but it is useful as a starting point for instance, for the hot spots estimation, and the definition of scenarios common between the safety (i.e. Step 2 and Step 3), and environmental sustainability assessments (Step 4).

Table B.1. Example of possible guiding questions to describe the chemical/material under assessment, the processes and product applications of the SSbD system under study

Chemical/material definition	**1.** Is the chemical/material known? **2.** If yes, provide the chemical/material identity information, for example: ☐ Name of the chemical/material (IUPAC name, trade name…) ☐ Composition ☐ Numerical identifiers (EC, CAS, INDEX, UFI, ERM….) ☐ Information related to molecular and structural formula ☐ Other
Processes related to the chemical/material under study	1. Are the production and processes known? **3.** If yes, select which of the following(s) better represent the process under study ☐ The chemical/material is consumed or used for chemical processing to be transformed into another chemical/material; ☐ The chemical/material is intentionally added as a component in a mixture/formulation process; ☐ The chemical/material is used in the manufacturing of a product and is not meant to be part of the final product; ☐ The chemical/material is used in the manufacturing of a product and is meant to be part of it; ☐ End of Life management (waste disposal or recovery) of the chemical/material. ☐ Other
Product application(s) related to the chemical/material under study	**4.** Is the final product/application known? **5.** If yes, define the final product/application(s) to the detail that is possible by for instance collecting the following information: ☐ The description of the product ☐ Industry sector of the product (if applicable) ☐ Function of the chemical/material in the product ☐ Product specific, safety, sustainability, and functional needs ☐ Other **6.** Based on the application, does/will the chemical/material under study follow specific requirements based on existing legislation? (e.g. food contact material, plastic packaging, cosmetics, Best Available Techniques, etc.)
Life cycle of the chemical/material under study	**7.** Draft of the life cycle of the chemical/material to assess (this includes the raw materials with suppliers, the downstream customers – if any, uses, and end-of-life) **8.** Based on the draft of the life cycle, define the system boundaries of your chemical/material study for the assessment
(re)design	**9.** Select one of the following options better representing the goal of the innovation: ☐ Development of a chemical/material → **Molecular (re)design** ☐ Development/Improvement of an application → **Product/application (re)design** ☐ Development/Improvement of a process → **Process (re)design**

Source: Own elaboration

Table B.2. Guiding questions to define the SSbD system under study specifically regarding the innovation. Some questions are in common for each level of the (re)design (molecular, process, and product), and others are more specifically for each of the three levels. [Please, note that the term "alternative technologies" refer to the general innovation under study. Alternative technologies for instance can refer either to alternative raw materials, production processes or alternative chemical/material, etc.]

Definition of the system for the alternative technology(ies)	**1.** What is the goal of your innovation and what are the design principles accompanying the fulfilment of the goal? (for instance, substitution of a SVHC, reduction of the water consumption during the chemical/material production process, etc) **2.** How many alternative technologies are you considering for your innovation goal? **3.** Is there any variation compared to the initial system to fulfil the function (e.g. different amount of chemical/material/formulation/mixture)?
Link to the (re)design phase and the design principle potentially adopted for the innovation	**4.** List all the design principles your innovation **5.** For each design principle provide the list of the indicators to assess the implementation of the design principles.
Preliminary study for the expected hotspots	**6.** Could you at this stage according to existing studies on the selected alternatives be able to preliminary identify potential hot spots? (e.g. water consumption, workers exposure) **7.** Could you at this stage identify the expected life cycle stage more affected by the innovation (either positively or negatively)?
Molecular (re)design	**8.** Is there any existing chemical/material that can be used as a reference to compare the results of the SSbD study? **9.** If no reference chemical/material has been selected, the reference might be chosen with one of the following aspects: ☐ Chemical/material with similar structure ☐ Chemical/material fulfilling the same function ☐ Representative Chemical/material as for the definition of Representative Product in the PEF method ☐ Other criteria to define the benchmark **10.** At which Technology Readiness Level (TRL) is chemical/material under development? (TRL 1-3 usually means laboratory scale, 4-6 pilot scale) Or are the alternatives already in the market?
Process (re)design	**11.** Does the improvement of the process require a new technology? **12.** If yes, at which Technology Readiness Level (TRL) is the new technology(ies) for the process improvement? (TRL 1-3 usually means laboratory scale, 4-6 pilot scale) Or are the alternatives already on the market? **13.** Provide information about the new technology needed for the improvement of the process, for instance the characteristics, the energy and auxiliaries consumed, its emissions and waste generated…
Product (re)design	**14.** Does the (re)design of the product/application involve a new application? **15.** If yes, at which Technology Readiness Level (TRL) is the new technology(ies) for the process improvement? (TRL 1-3 usually means laboratory scale, 4-6 pilot scale) Or are the alternatives already on the market? **16.** Provide information about the new technology needed for the improvement of the product/application

Source: Own elaboration

Annex C. Decision-making

Performing the whole SSbD assessment at each phase of the innovation process can be resource consuming. Is it possible to prioritise some aspects of the SSbD assessment?

[Examples are provided as exploratory phase for methodologies supporting the decision making]

Yes, some aspects may be prioritised when considering the specificity of your innovation case (e.g. level of innovation, market) and its goal, there may be aspects that are more relevant at different stages or that your organisation considers as a priority.

To determine these aspects, you can develop a ranking by using different methodologies. One of most widely used tools for decision-making and prioritisation/ranking is the Analytic Hierarchy Process (AHP) (Saaty, 1987) 1980). The primary goal of the AHP is to select an alternative that best satisfies a given set of criteria out of a set of alternatives or to determine the weights of criteria in any application. This methodology can be structured in five main steps that are:

I. State the decision problem/goal,

II. Identify the criteria/sub-criteria that influence the goal and the different alternatives for reaching the decision goal,

III. Structure the problem in a hierarchy of different levels (goal, criteria, sub-criteria, alternatives),

IV. Compare each element in the corresponding level and calibrate them on the numerical scale,

V. Perform consistency checks and calculations to achieve the final decision.

This method relies on a pairwise comparison of the relative importance of two criteria, and uses a nine-point scale for the assessment of each pair of criteria, where “1” implies equal importance between two criteria and “9” indicates the absolute importance of one criterion over another (Table C.1). A pairwise comparison matrix CxC is formed, where C is the number of elements to be compared. Note that this can be applied to both qualitative and quantifiable criteria, and it is done by experts in the domain. Box 4 shows an example of this application.

The main advantages of the AHP are the use of simple algebra, the adaptability of the model for different problems, the ability to use for quantitative and qualitative information, the possibility to be used by multidisciplinary experts, the ability to measures consistency of judgements, and its very wide range of usage fields. On the other hand, the disadvantages are the high computational requirement even for small problems (the number of pair comparisons performed), the assumption of criteria independence, ordering the judgement alternatives when a new judgement alternative is added can be challenging, and its (at least, in poart) subjective nature (Ishizaka & Labib, 2009).

Table C.1. Pairwise comparison of the relative importance of two criteria with nine-point scale for the assessment of each pair of criteria, where “1” implies equal importance between two criteria and “9” indicates the absolute importance of one criterion over another

Intensity of importance	Definition
1	Equal importance
3	Moderate importance
5	Strong importance
7	Very strong importance
9	Absolute importance
2, 4, 6, 8	For compromise between the above values

Source: Own elaboration

Box 4. Example to determine the weights of three different criteria for certain application

The example shows how to calculate the priority vector (PV), which is the overall weighting for each criterion. We start with the calculation of the relative weight for each of the 3 criteria consider and we calculate the total as the sum of the values by column.

Table C.2. Decision making: example of the weight for the 3 criteria

Criteria	C1	C2	C3
C1	1	5	4
C2	1/5	1	1/3
C3	1/4	3	1
Total	1.45	9	5.33

Source: Own elaboration

Secondly, we calculate the normalised value by dividing each value by the total.

Table C.3. Decision making: normalised value of the weighted criteria

Criteria	C1	C2	C3
C1	1/1.45=0.69	0.56	0.75
C2	0.2/1.45=0.14	0.11	0.06
C3	0.17	0.33	0.19

Source: Own elaboration

Finally, we calculate PV using the arithmetic mean (depending on the method it is also done with the geometric mean) that will be the weighted score suggested for each criterion:

Table C.4. Decision making: PV using the arithmetic mean

Criteria	C1
C1	**0.67**
C2	**0.10**
C3	**0.23**

Source: Own elaboration

Consistency checks are key in the process since the consistency of the judgements is not guaranteed due to the subjective judgements by the experts. This is mainly done through a consistency ratio (CR) computation (consistency index (CI) divided by the random consistency index (RI) that depends on the number of criteria being 0.58 for n=3, 0.9 for n=4, etc.) with a threshold of 0.1 that once it is exceeded, initial judgments must be revised by the experts:
λ is the principal Eigen Value and is calculated through first of all, a matrix multiplication of the pairwise comparison and the PV, and then dividing the result matrix by the PV values and calculating the average of these values. In this case the λ equals 3.087 and the CI equals 0.043. Thus, the CR equals 0.07 ≤ 0.01, being the judgement valid

Which approach or methodologies are available to decide among different alternatives when several aspects are considered in the assessment?

[Examples are provided as exploratory phase for methodologies supporting the decision making]

Ranking/selecting among different alternatives considering several aspects (i.e. Multi-Criteria Decision Making - MCDM) usually requires an analysis of several different types of complex problems and thus, no method or process is recommended as a better choice. Specific methods might apply to different problems, and the decision maker has to select the method that best fits the problem at hand (Munier & Hontoria, 2021).

Generally, MCDM can be divided into two main categories based on the number of alternatives (Taherdoost & Madanchian, 2023). The first one is multi-objective decision making (MODM) with innumerable alternatives (i.e., with infinite admissible answers within a continuous decision space) that addresses an optimization problem with no direct and specific alternative chosen as a solution. The second one is multi-attribute decision making (MADM) with numerable alternatives (i.e. with finite admissible answers within a discrete problem) that addresses an evaluation problem of choosing the (best) solution between a discrete number of alternatives.

Generally, MCDM can be divided into two main categories based on the number of alternatives (Taherdoost & Madanchian, 2023). The first one is multi-objective decision making (MODM) with innumerable alternatives (i.e., with infinite admissible answers within a continuous decision space) that addresses an optimization problem with no direct and specific alternative chosen as a solution[4]. The second one is multi-attribute decision making (MADM) with numerable alternatives (i.e. with finite admissible answers within a discrete problem) that addresses an evaluation problem of choosing the (best) solution between a discrete number of alternatives.

- Analytic Hierarchy Process (AHP) (Saaty, 1987) that uses pairwise comparisons of hierarchical criteria considering different information.
- Data Envelopment Analysis (DEA) (Charnes et al., 1978) that is used in specific cases for performance evaluation or benchmarking where no subjective inputs are required. The combination of LCA and DEA methodologies can be employed to assess eco-efficiency of a wide spectrum of production systems (Laso et al., 2022).
- Fuzzy Set Theory (FST) (Goguen, 1973) that is used to address the uncertainty in human beliefs and quantify the linguistic facet of accessible data and preferences linked to subjective and ambiguous problems.
- Technique for Order Preference by Similarity to Ideal Solutions (TOPSIS) (Hwang & Yoon, 1981) that makes an evaluation based on the distance of the alternatives to the ideal solution.
- Goal Programming (GP) (Charnes & Cooper, 1957) that search to solve problems with multiple, conflicting objectives with a balance of the trade-offs between them by minimizing the derivation of each objective from the desired target.

Getting in touch with the EU

In person

All over the European Union there are hundreds of Europe Direct centres. You can find the address of the centre nearest you online (european-union.europa.eu/contact-eu/meet-us_en).

On the phone or in writing

Europe Direct is a service that answers your questions about the European Union. You can contact this service:

— by freephone: 00 800 6 7 8 9 10 11 (certain operators may charge for these calls),

— at the following standard number: +32 22999696,

— via the following form: european-union.europa.eu/contact-eu/write-us_en.

Finding information about the EU

Online

Information about the European Union in all the official languages of the EU is available on the Europa website (european-union.europa.eu).

EU publications

You can view or order EU publications at op.europa.eu/en/publications. Multiple copies of free publications can be obtained by contacting Europe Direct or your local documentation centre (european-union.europa.eu/contact-eu/meet-us_en).

EU law and related documents

For access to legal information from the EU, including all EU law since 1951 in all the official language versions, go to EUR-Lex (eur-lex.europa.eu).

EU open data

The portal data.europa.eu provides access to open datasets from the EU institutions, bodies and agencies. These can be downloaded and reused for free, for both commercial and non-commercial purposes. The portal also provides access to a wealth of datasets from European countries.

Science for policy

The Joint Research Centre (JRC) provides independent, evidence-based knowledge and science, supporting EU policies to positively impact society

EU Science Hub
joint-research-centre.ec.europa.eu

Publications Office
of the European Union