Safe and sustainable by design chemicals and materials: framework for the definition of criteria and evaluation procedure for chemicals and materials

Carla Caldeira, Irantzu Garmendia, Lucian Farcal, Lucia Mancini, Davide Tosches, Antonio Amelio, Kirsten Rasmussen, Hubert Rauscher, Juan Riego Sintes, Serenella Sala

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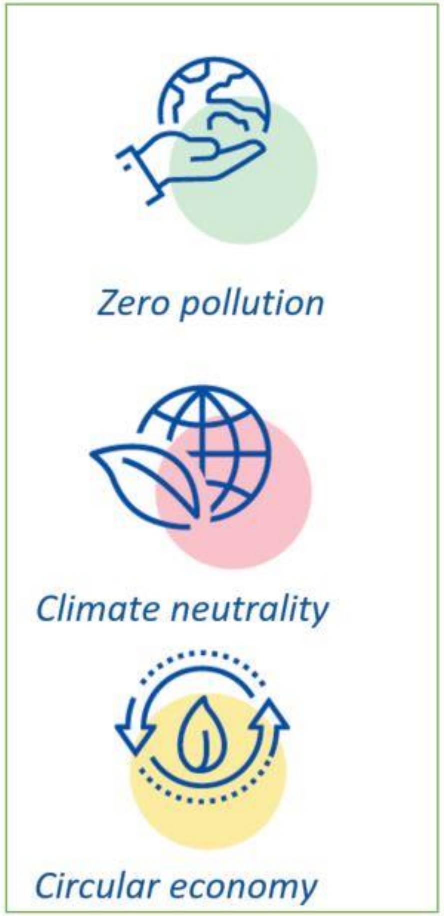
References

- European Commission, Joint Research Centre, Caldeira, C., Farcal, R., Moretti, C., et al., Safe and sustainable by design chemicals and materials: review of safety and sustainability dimensions, aspects, methods, indicators, and tools, Publications Office of the European Union, 2022, https://data.europa.eu/doi/10.2760/879069
- European Commission, Joint Research Centre, Caldeira, C., Farcal, L., Garmendia Aguirre, I., et al., Safe and sustainable by design chemicals and materials: framework for the definition of criteria and evaluation procedure for chemicals and materials, Publications Office of the European Union, 2022, https://data.europa.eu/doi/10.2760/487955

Introduction

Policy context

The EU Green Deal



Chemicals Strategy for Sustainability (CSS)

- phase out the **most harmful substances** and
- substitute, as far as possible, **substances of concern**, and otherwise minimise their use and track them

Novel approaches to analysing and comparing, across all life cycle stages, effects, releases and emissions for specific chemicals, materials, products and services, and move towards zero-pollution for air, water, soil and biota.

CSS Action Plan

Develop **safe and sustainable-by-design (SSbD)** criteria for chemicals and materials

https://environment.ec.europa.eu/strategy/chemicals-strategy_en

SSbD in the EU CSS

- ***Safe and sustainable by design can be defined*** *as a pre-market approach to chemicals and materials design that focuses on providing a function (or service), while* ***avoiding volumes and chemical and material properties that may be harmful to human health or the environment, in particular groups of chemicals likely to be (eco)toxic, persistent, bio-accumulative or mobile.***

- *Overall sustainability should be ensured by minimising the environmental footprint of chemicals and materials in particular in relation to* ***climate change, resource use, and protecting ecosystems and biodiversity, adopting a lifecycle perspective.***

(Definition adapted from EU Chemicals Strategy for Sustainability).

Framework to define safe and sustainable by design **(SSbD) criteria for chemicals and materials** that should **contribute to achieve the CSS ambitions**, **beyond current regulatory compliance.**

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://ec.europa.eu/environment/strategy/chemicals-strategy_en

European Commission

Objectives of the framework

- **Promoting the application of the Safe and Sustainable by Design** approach to chemicals and materials
- **Steering innovation** towards the green industrial transition, resulting in the EU becoming a global reference for safety and sustainability targets;
- **Providing guidance** on criteria development for the design of ‘safe’ and ‘sustainable’ chemicals/materials;
- **Driving innovation** towards the substitution or minimisation of the production and use of substances of concern, in line with and beyond upcoming regulatory obligations;
- **Minimising or, as far as possible, eliminating the impact on human health, climate and the environment** (air, water, soil) along the entire chemical’s and material’s life cycle;
- **Enabling comparative assessment of chemicals and materials** based on safety and sustainability performance for a given function or application context.

European Commission

Definitions and sustainability dimensions in the proposed SSbD framework

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Definitions: safety and sustainability

- The **sustainability** concept is complex and multifaceted. The general definition is related to the original definition of sustainable development: the **development that meets the needs of the present without compromising the ability of future generations to meet their own needs.** Hence, ensuring that any human actions remains far from irreversibility (in terms of loss of resources of impacts to the environment) and consider present and future conditions.

- When applied in the context of chemicals/materials, the concept of **sustainability** could be formulated as **the ability of a chemical/material to deliver its function without exceeding environmental and ecological boundaries along its entire life cycle, while providing welfare, socio-economic benefits and reducing externalities.**

- The **safety** concept is transversal to all sustainability dimensions (environmental, social and economic) and it is related to the absence of unacceptable risk (in line with REACH art 68) for humans and the environment, **preferably ensured by avoiding chemicals with intrinsic hazard properties**.

European Commission

Dimensions in the proposed framework

- Sustainability dimensions:
  - Safety
  - Environmental
  - Social
  - Economic
- The proposed SSbD framework addresses **safety and environmental dimensions and,** with less detail, **the social and economic ones**

Definitions: ‘By-design’ (re-design)

In the context of SSbD criteria definition for chemicals and materials, the term ‘by-design’ can be interpreted at 3 levels:

- **Molecular design**: this is the design of new chemicals and materials based on the atomic level description of the molecular system. This type of design effectively delivers new substances, whose properties may, in principle, be tuned to be safe(r) and (more) sustainable.

- **Process design**: this is the design of new or improved processes to produce chemicals and materials. Process design does not change the intrinsic properties (e.g. hazard properties) of the chemical or material, but it can make the production of the substance safer and more sustainable (e.g. more energy or resource efficient production process, minimising the use of hazardous substances in the process). The process design includes upstream steps, such as the selection of the feedstock.

- **Product design**: this is the design of the product in which the chemical/material might be used with a specific function that will eventually be used by industrial workers, professionals or consumers.

The SSbD framework proposed in this report covers all three levels. It can be used **to determine into which direction molecular design should go** (including designing an optimal production process), but it is also intended to be useful for the engineers and scientists improving or inventing **new production processes (re-design)** for already existing chemicals and materials, and for product designers, when they need e.g. **to select different chemicals and materials to meet the functional demands of the product under development**.

Components of the SSbD framework

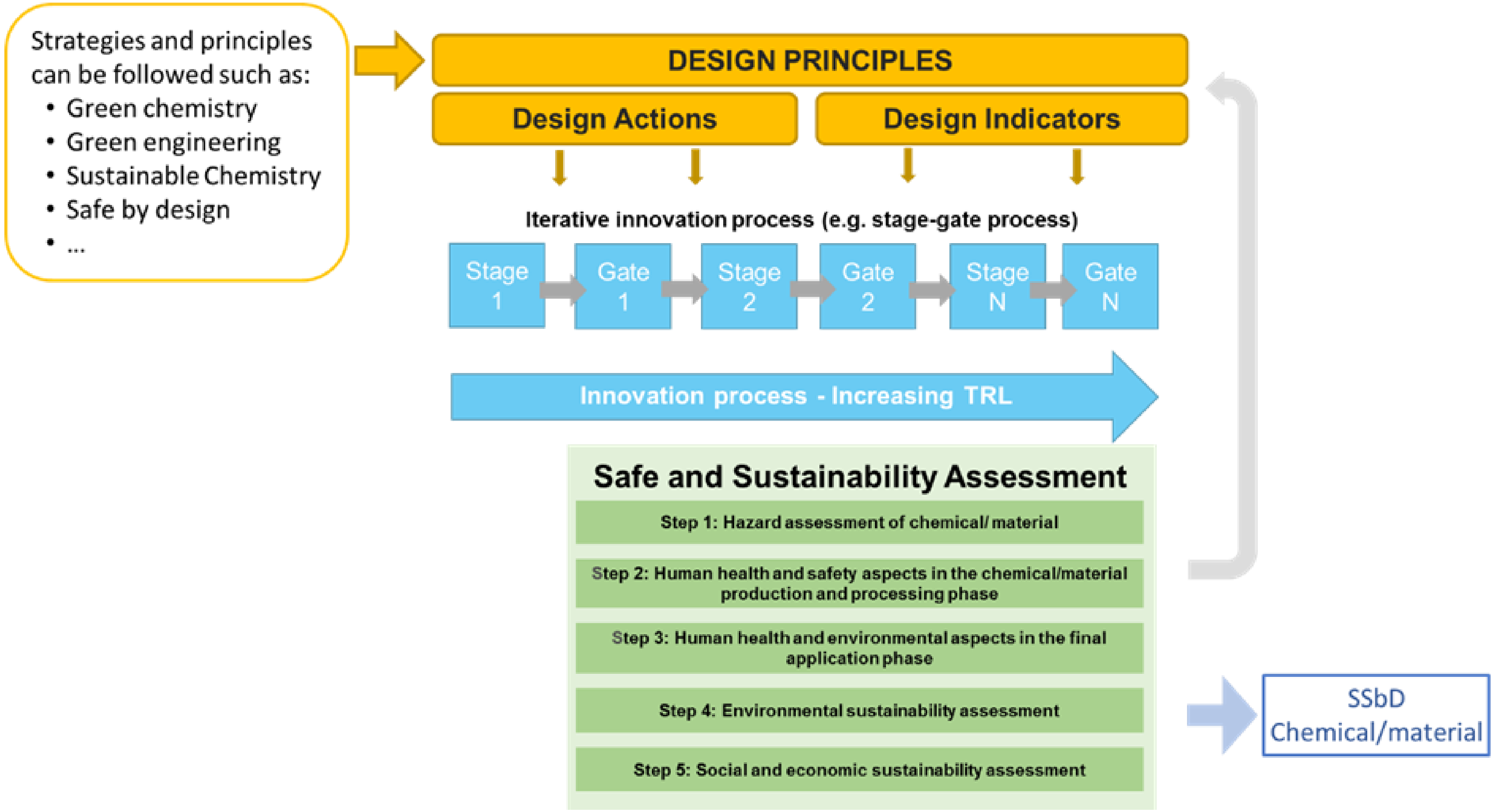
- To support the development of a SSbD chemical/material, certain principles should be followed in the design phase.
- SSbD framework entails two components:

1. a **(re)design phase** in which design guiding principles and indicators are proposed to support the design of chemicals and materials, and
2. a **safety and sustainability** assessment phase in which the safety, environmental and socio-economic sustainability of the chemical/ material are assessed. Socio-economic aspects are included in the framework to be explored as methods still need to be further developed.

SSbD framework components

Integration of SSbD in the innovation cycle including **principles to be considered in the design phase** of SSbD chemicals and materials

Safety and sustainability performance is verified with the **assessment** allowing the classification of the chemical/material as SSbD.



TRL: Technology Readiness Level)

Structure of the framework: a stepwise approach

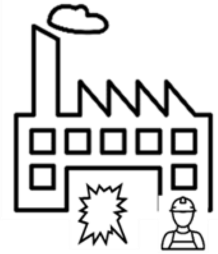
Safety and sustainability assessment

Safety and sustainability components captured in the framework with the illustration of the **life cycle stages covered** and the **subject of the assessment**

Hazard properties of the chemical/material

- The assessment focuses on the **hazard properties** (human health, environmental and physical hazards) of chemicals and materials
- The assessment addresses the following aspects: **human health hazards, environmental hazards and physical hazards**

Hazards and risks related to the chemical/material production and processing

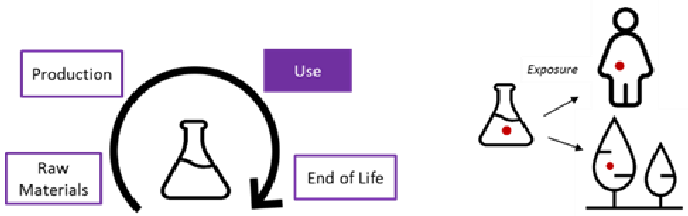


- **Human health and safety aspects** related to the chemical/material production and processing are assessed.
- It refers to **production process** from the raw material extraction (from natural resources) to production (e.g. substance manufacturing, mixing) of the chemical/material including the recycling or waste management

Safety and sustainability assessment

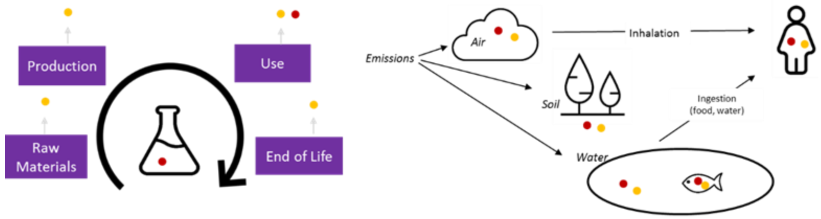
Safety and sustainability components captured in the framework with the illustration of the **life cycle stages covered** and the **subject of the assessment**

Hazards and risks related to the chemical/material application



- The **health and environmental** aspects related to the chemical/material final application are assessed.
- It refers to **use-specific exposure** to the chemical/material and the associated risks

Environmental impacts along the entire chemical/material life cycle



- This step covers other **environmental sustainability aspects** along the life cycle by means of LCA
- The assessment addresses the environmental footprint (EF) impact categories at the level of **toxicity, climate change, pollution and resources**

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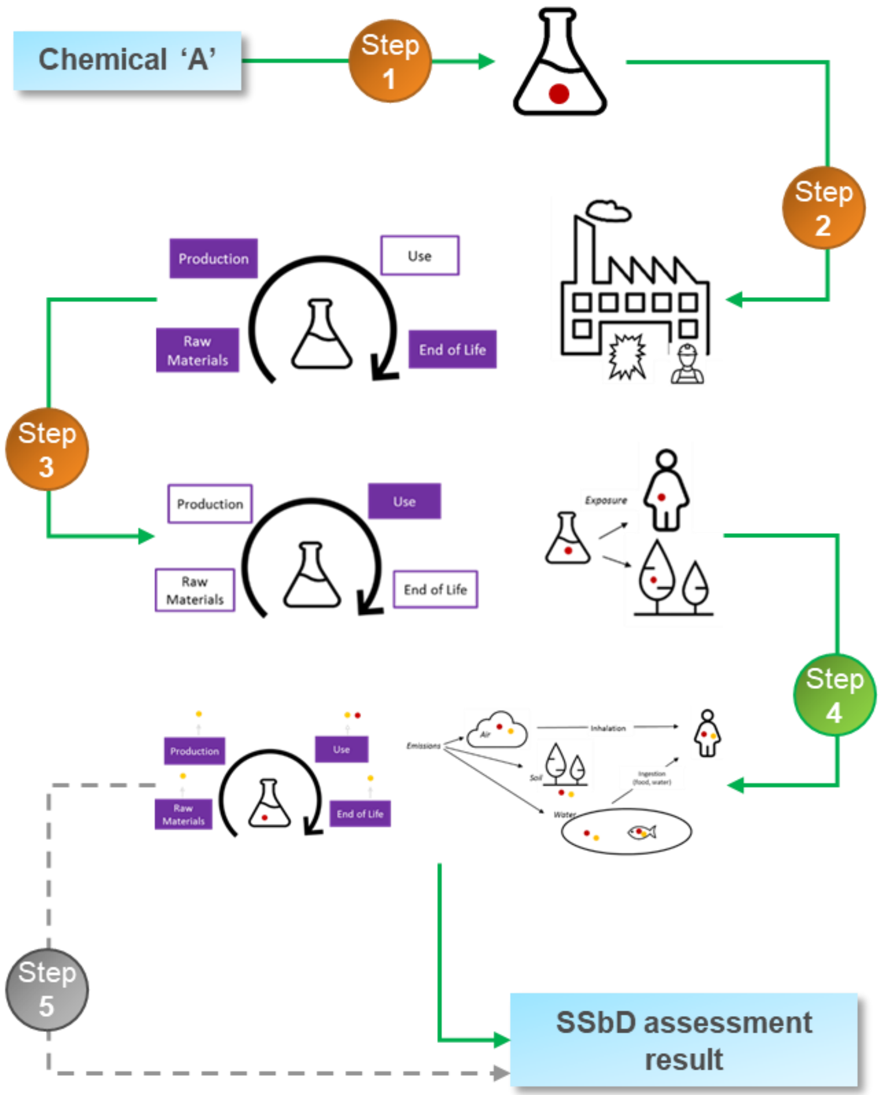
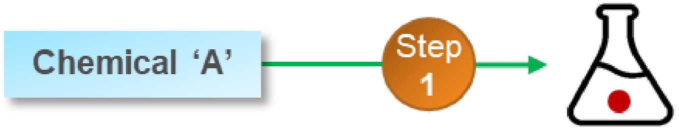
Methodology for criteria definition

- For each step the methodology refers to:
  - a detailed description of **which aspects and indicators** that can be used to measure such aspects and respective **method**,
  - a proposal for the **definition of criteria** for each of the aspect and
  - an **evaluation procedure**.



Step 1 - Hazard assessment of the chemical/material

- This step looks at the intrinsic properties of the chemical or material in order to understand its hazard profile before further assessing the safety during use.
- The goal is to identify the most appropriate criteria that can be applied during the design (or re-design) of chemicals and materials in order to align with the overall objectives of the CSS, e.g.:
  - Ensure that all chemicals and materials placed on the market are in themselves safe and that they are produced and used safely and sustainably*
  - Ensure that final products do not contain the most harmful substances
  - Drive the substitution of the substances of concern



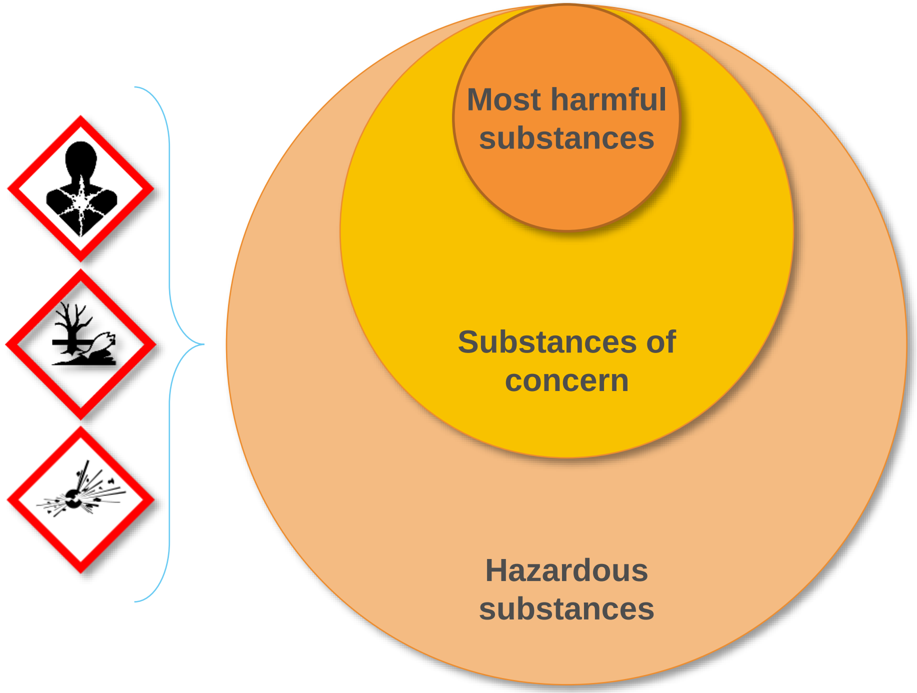
*point covered also by other components of the framework

Step 1

Aspects and indicators

- Generally, the methodology for criteria definition follows the specifications and criteria established in CLP and REACH regulations, as well as CSS and SPI

- In the EU chemicals legislation, three main hazard classes are described and these classes are also included in the SSbD framework:
  - Human health hazards
  - Environmental hazards
  - Physical hazards
- Based on the hazard properties, three main groups of substances were defined (*aligned to CSS and SPI*):
  - Most harmful substances
  - Substances of concern
  - Other hazard classes



__CLP__ = Regulation (EC) No 1272/2008; __REACH__ = Regulation (EC) No 1907/2006; __CSS__ = EU Chemicals Strategy for Sustainability Towards a Toxic-Free Environment (COM (2020) 667); __SPI__ = Proposal for a Regulation establishing a framework for setting ecodesign requirements for sustainable products (COM(2022 142 final))

Aspects and indicators

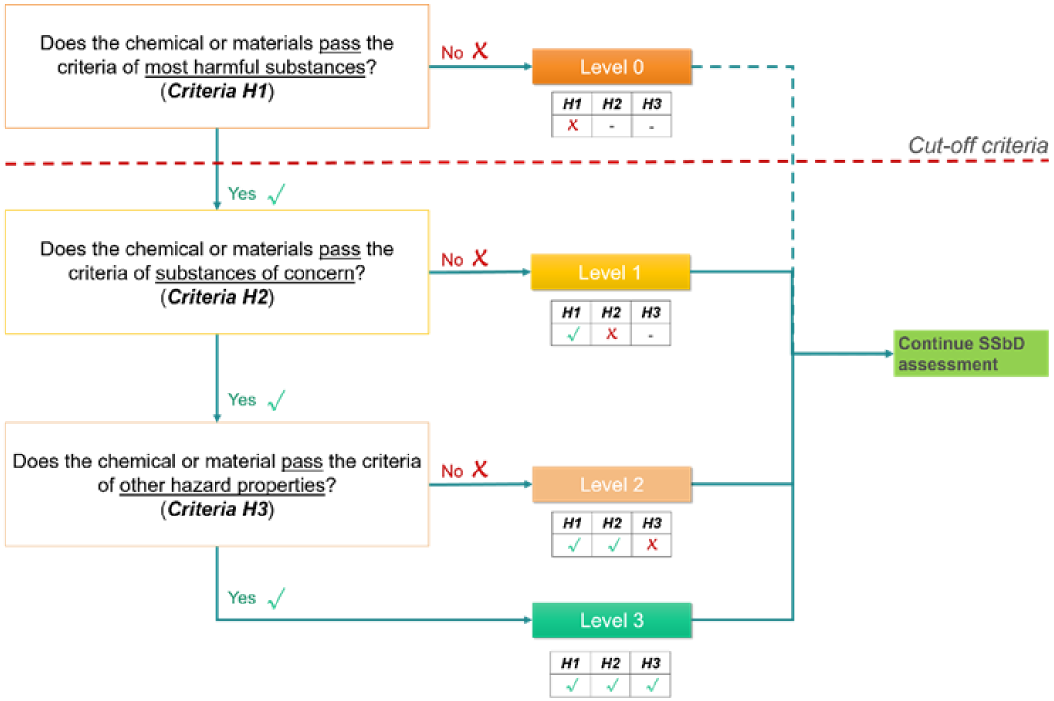
Group definition	Human health hazards	Environmental hazards	Physical hazards	
Includes the most harmful substances (according to CSS), including the substances of very high concern (SVHC) according to REACH Art. 57(a-f).	❑ Carcinogenicity Cat. 1A and 1B ❑ Germ cell mutagenicity Cat. 1A and 1B ❑ Reproductive / developmental toxicity Cat. 1A and 1B ❑ Endocrine disruption Cat. 1 (human health) ❑ Respiratory sensitisation Cat 1 ❑ Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 1, including immunotoxicity and neurotoxicity	❑ Persistent, bioaccumulative and toxic / very persistent and very bioaccumulative (PBT/vPvB) ❑ Persistent, mobile and toxic / very persistent and mobile (PMT/vPvM) ❑ Endocrine disruption Cat. 1 (environment)		Criterion **H1**
Includes substances of concern, as described in CSS, defined in the Article 2(28) of SPI proposal and that are not already included in Criterion H1.	❑ Skin sensitisation Cat 1 ❑ Carcinogenicity Cat. 2 ❑ Germ cell mutagenicity Cat. 2 ❑ Reproductive / developmental toxicity Cat. 2 ❑ Specific target organ toxicity - repeated exposure (STOT-RE) Cat. 2 ❑ Specific target organ toxicity - single exposure (STOT-SE) Cat. 1 and 2 ❑ Endocrine disruption Cat. 2 (human health)	❑ Hazardous for the ozone layer ❑ Chronic environmental toxicity (chronic aquatic toxicity) ❑ Endocrine disruption Cat. 2 (environment)		Criterion H2
Includes the other hazard classes not part already in Criteria H1 and H2.	❑ Acute toxicity ❑ Skin corrosion ❑ Skin irritation ❑ Serious eye damage/eye irritation ❑ Aspiration hazard (Cat. 1) ❑ Specific target organ toxicity - single exposure (STOT-SE) Cat. 3	❑ Acute environmental toxicity (acute aquatic toxicity)	❑ Explosives ❑ Flammable gases, liquids and solids ❑ Aerosols ❑ Oxidising gases, liquids, solids ❑ Gases under pressure ❑ Self-reactive ❑ Pyrophoric liquids, solid ❑ Self-heating ❑ In contact with water emits flammable gas ❑ Organic peroxides ❑ Corrosivity ❑ Desensitised explosives	Criterion H3

Step 1

Evaluation system

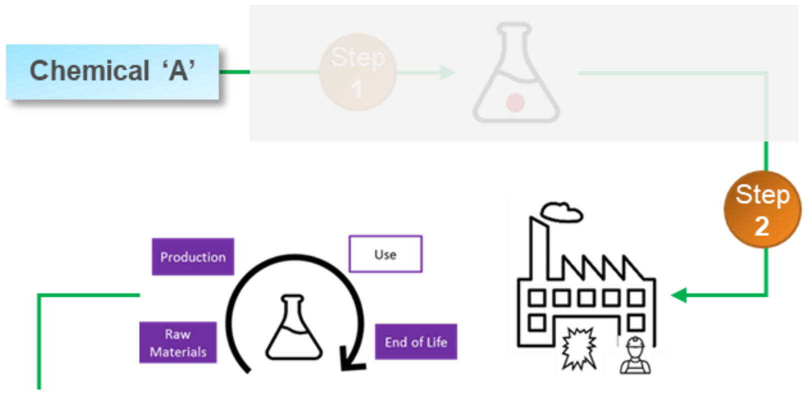
- The chemicals or materials that pass a certain criterion of Step 1 will get a ‘level’ that reflects the result of the hazard profile related to aspects included in that specific criterion.
- Four levels are proposed:
  - **Level 0** - chemicals or materials that do not pass hazard criterion H1 (e.g. considered most harmful substances)
  - **Level 1** - chemicals or materials that pass hazard criterion H1 but do not pass criterion H2 (e.g. induce chronic effects, part of the substances of concern)
  - **Level 2** - chemicals or materials that pass hazard criteria H1 and H2 but do not pass criterion H3 (e.g. with other hazard properties)
  - **Level 3** - chemicals or materials that pass all safety criteria in Step 1.

For Level 3 chemicals or materials that are not classified according to their intrinsic properties and CLP criteria, it should be recognised that the chemical/material could still pose risk in certain applications.



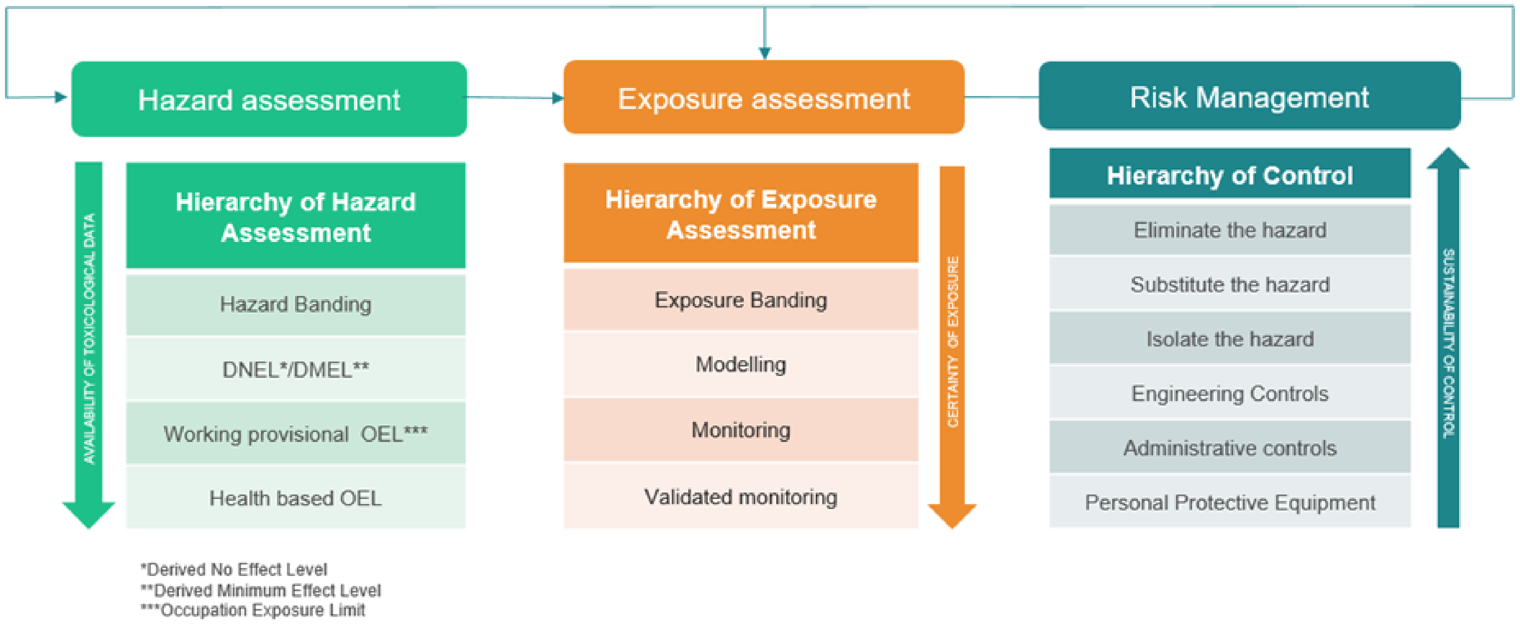
Step 2 - Human health and safety aspects in the chemical/material production and processing phase

- In this step, the human health and safety aspects related to the chemical/material production and processing are assessed.
- Incudes occupational safety and health (OSH) aspects in the life cycle of the chemical/material.
- It refers to production production of the chemical/material (considering precursors...), the processing (mixing, compounding, transforming...) including the recycling or waste management.



Aspects and indicators

- The aspects included refer to the human health and safety during the production and processing of chemical/material.
- The risk should be estimated as a combination of the chemical/material hazards and the exposure during the different processes process and the Risk Management Measures (RMMs) already in place to control the risks.



Hierarchy for a tiered risk assessment depending on the data availability for each of the aspects (Laszcz-Davis et al., 2014)

Step 2

Aspects and indicators

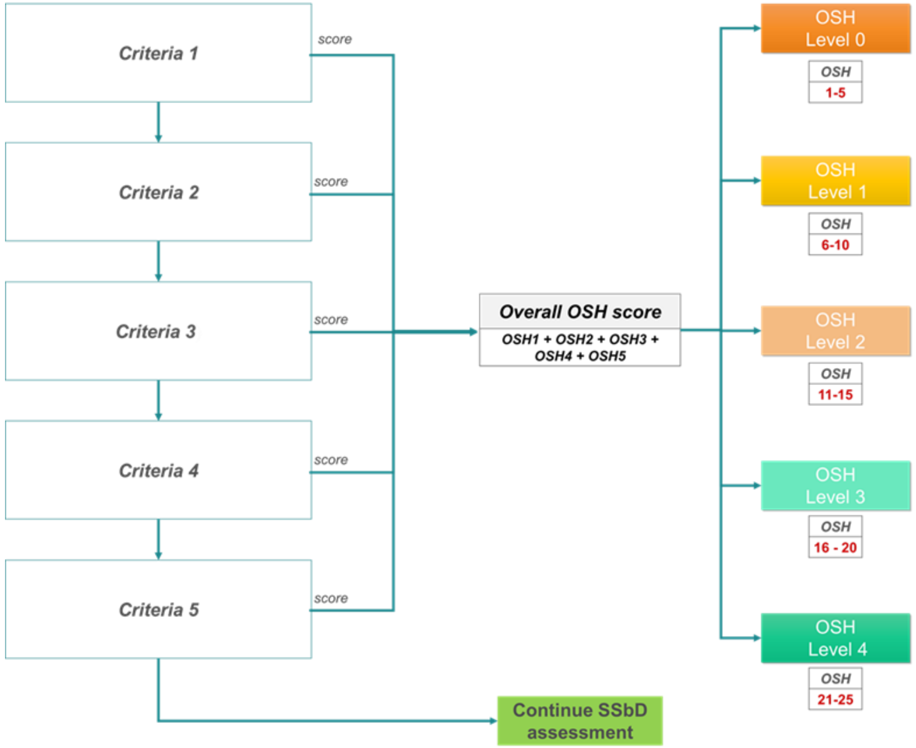
- There are different qualitative/simplified models available (also known control banding models) for the safety assessment and management at the workplace.
- These models are designed to characterise the risk at the workplace in a Tier 1 approach, when the whole set of data to perform a quantitative assessment is not available.
- These models are based on assigning scores or levels to some of the following variables to be taken into account during the risk characterisation:
  - Hazards of chemicals
  - Exposure frequency and duration
  - Amount of chemical used or present
  - Physical properties of the chemical like volatility and dustiness
  - Operational conditions
  - Type of existing RMMs
  - Others

Step 2

Criteria definition and evaluation system

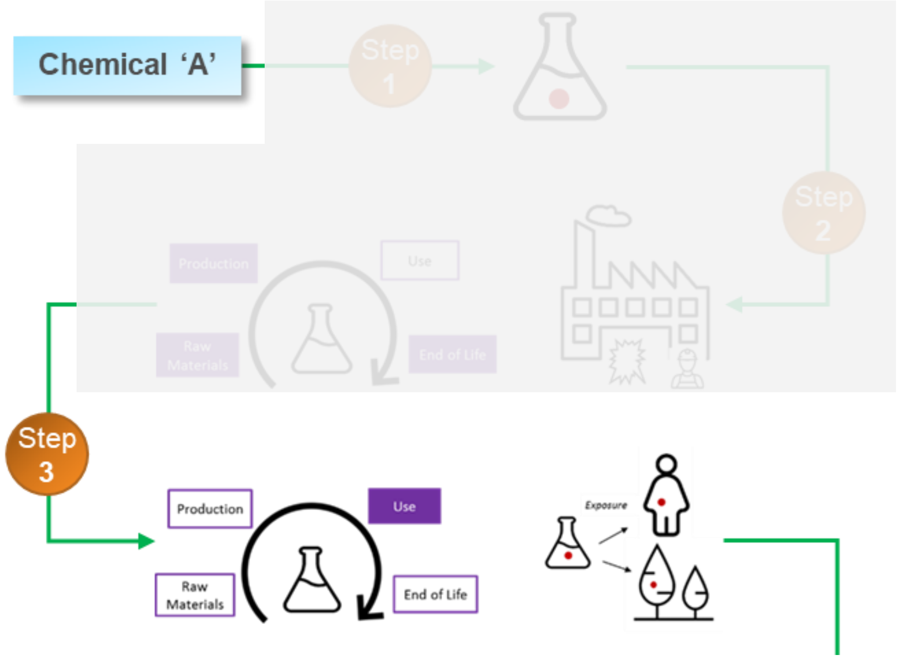
- From the aspects to be considered in Step 2, a set of criteria can be defined in order to assess the hazard and exposure aspects to estimate the risks from all the processes along the life cycle.
- The criteria will address the use of hazardous chemicals/materials as well as the process related potential of exposure.

Criteria 1	Criteria 2	Criteria 3	Criteria 4	Criteria 5	Safety	
4	4	5	5	5	21-25	Negligible risk
3	3	4	4	5	16-20	Low-risk
1	2	3	3	4	11-15	Medium-risk
1	1	2	2	3	6-10	High-risk
1	1	1	1	1	0-5	Very high risk



Step 3 - Human health and environmental aspects in the final application phase

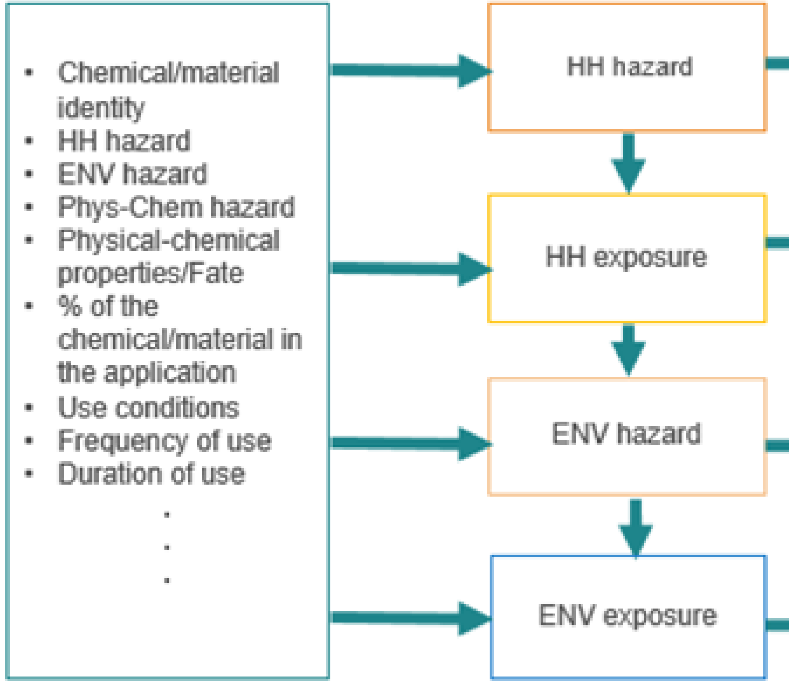
- In this step, the hazards and risks related to the chemical/material final application are assessed.
- It refers to use-specific exposure to the chemical/material and the associated risks.
- The goal is to assess whether the use of chemical/material in the final application poses any risk to the human health and the environment.



Step 3

Aspects and indicators

- The aspects are related to the human health and environment during the application of the chemical/material.
- The risk is characterised as a combination of the chemical/material hazards and the exposure assessment to the human health and the environment during the application.
- Information on the substance/material's intrinsic properties are necessary for the safety assessment.
- Other physical-chemical properties (e.g. physical form, vapour pressure, water solubility, octanol water partition coefficient) are also needed to identify the fate of the chemical/material, estimate the exposure path and characterise the risk.
- For the exposure estimation, it is particularly important to identify/describe the application and define the use conditions providing information on, frequency and duration of the exposure, amount of chemical/material used or present in the application, use conditions and use instructions.



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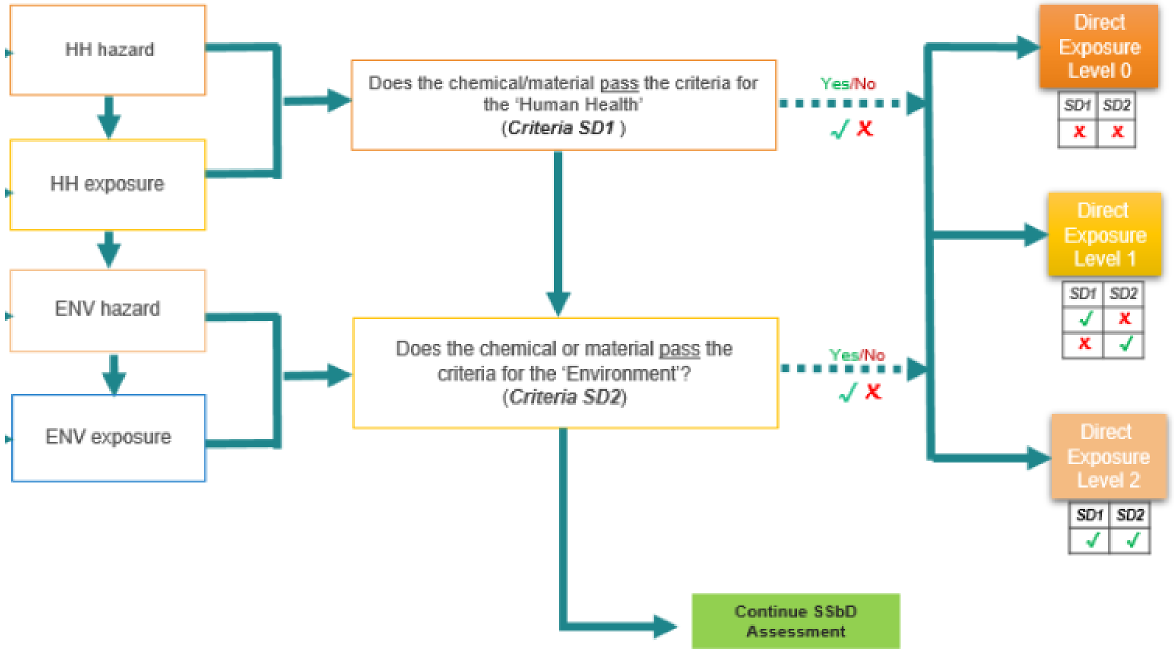
Step 3

Criteria definition and evaluation system

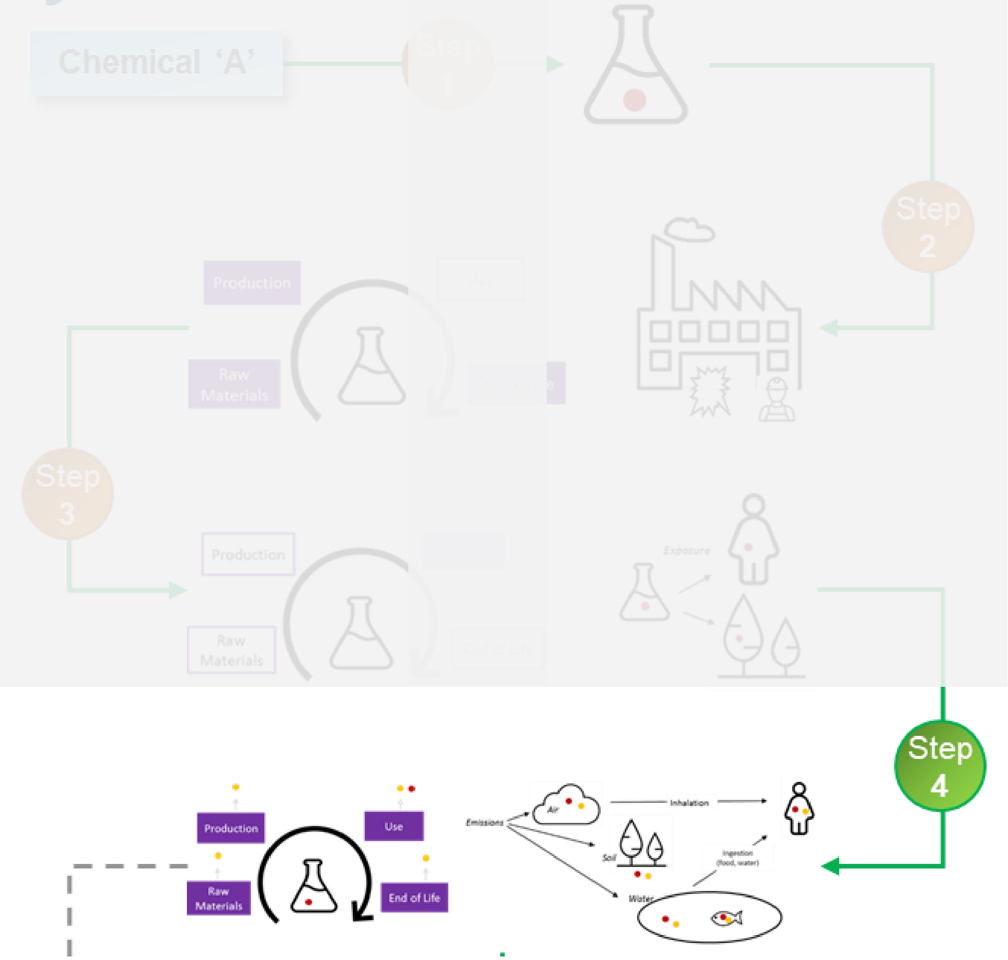
- A set of criteria can be defined to assess the human health and environment aspects.
- Once criteria are defined different safety levels can be defined both for the human health and the environment and a score and a colour code can be assigned to determine whether the criterion is considered as passed or not:

Position to safe level	Score	Colour code	Criteria evaluation
> Safe level + 50%	0		Fail the criteria
>Safe level; < safe level +50%	1		
>Safe level - 25% ; < Safe level	2		Pass the criteria
>safe level -50% ; <Safe level - 25%	3		
< Safe level – 50%	4		



Step 4 - Environmental sustainability assessment

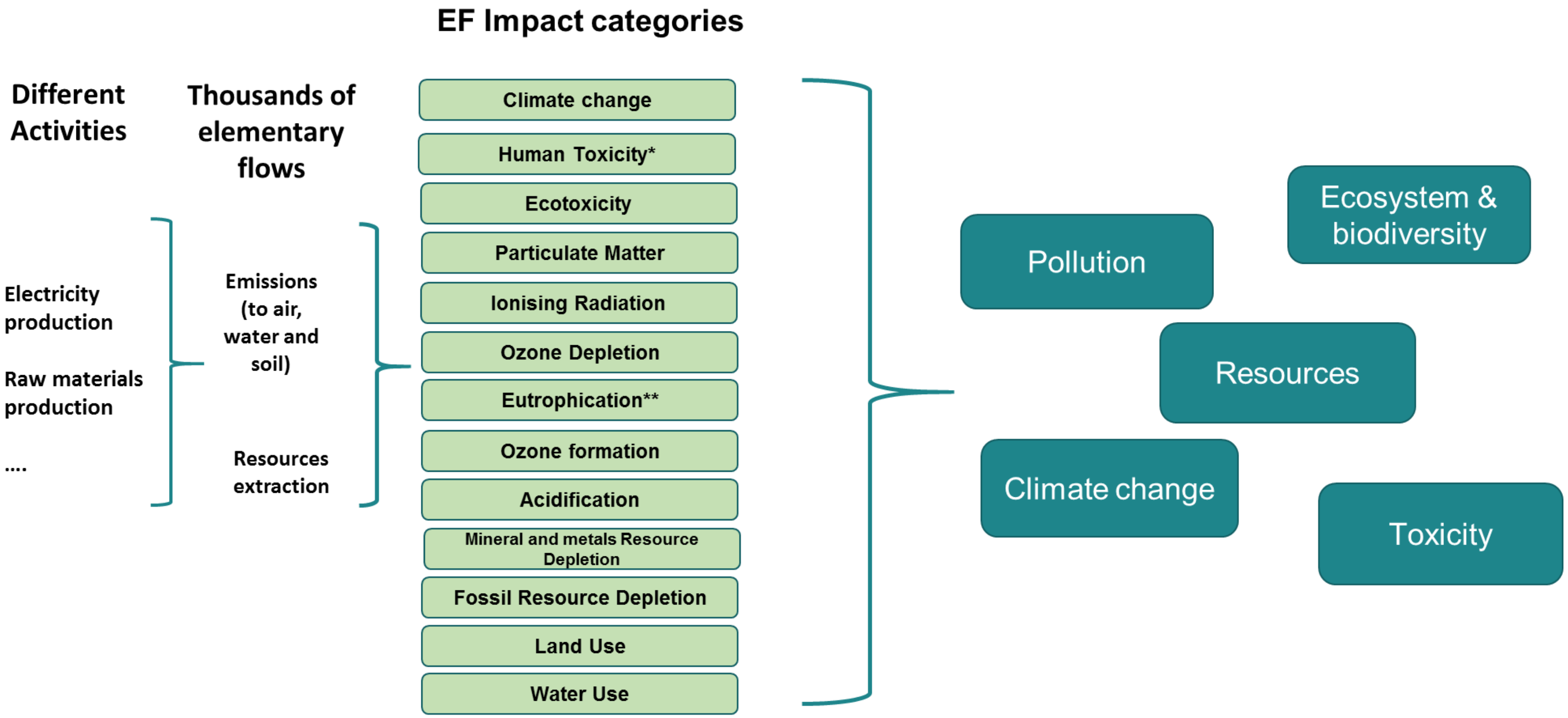
- This step covers **environmental impacts along the entire chemical/material life cycle**
- The CSS calls for the development of **SSbD criteria for chemicals** to be defined through a holistic framework integrating the minimisation of the environmental footprint of chemicals with their safety, circularity, and functionality **throughout their entire lifecycle**.
- **Life cycle assessment (LCA**) is proposed as a method to assess the environmental impacts of chemical production, use and end of life.



Step 4

Aspects and indicators

- Impact categories considered in the Environmental Footprint Impact Assessment method recommended by the European Commission to be used to measure the life cycle environmental performance of products
- The method considers in total 16 impact categories that are related to several policy objectives such as protection of human health and of biodiversity



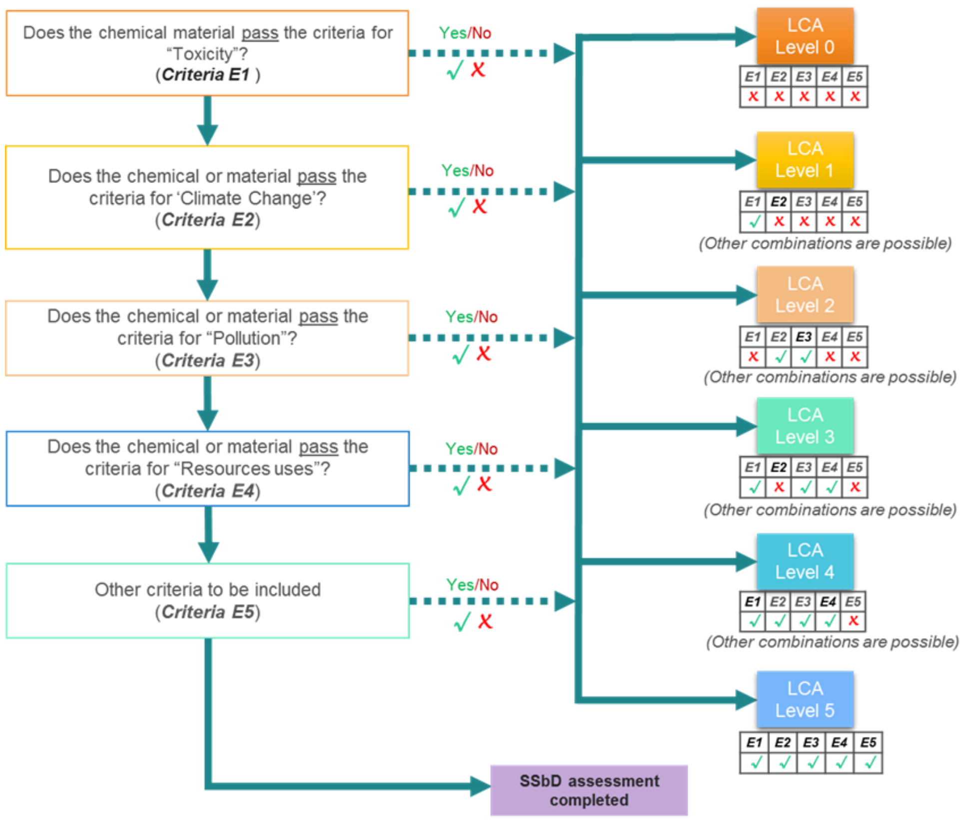
Criteria definition and evaluation system

- For each impact category a criterion should be defined as **a reduction of the impact category value of X% (target) relative to a reference value.**
- Once the criteria for each impact category are defined one can assess the chemical/material attributing a score
- For example, if the chemical/material shows no improvement relatively to the reference it would score 0, instead if the improvement is higher than 40% it would score 4
- The chemical/material that pass a certain criterion will get a ‘level’.

Position to reference	Score	Colour code	
No improvement	0		Fail the criteria
Improvement + 5%	1		
Improvement + 5% to 20%	2		Pass the criteria
Improvement + 20% to 40%	3		
Improvement > 40%	4		

Step 4

Criteria definition and evaluation system



LCA Assessment level (max score)	Aspect	Score	Level
Toxicity ES1 (max 12)	Human Toxicity, cancer	3	✗
	Human Toxicity non cancer	2	
	Ecotoxicity	1	
Climate Change ES2 (max 4)	Climate Change	3	✓
Pollution ES3 (max 32)	Ozone depletion	4	✗
	Particulate matter/Respiratory inorganics	2	
	Ionising radiation, human health	2	
	Photochemical ozone formation	1	
	Acidification	0	
	Eutrophication, terrestrial	4	
	Eutrophication, aquatic freshwater	3	
	Eutrophication, aquatic marine	2	
Resources ES4 (max 16)	Land Use	4	✓
	Water use	2	
	Resource use, minerals and metals	2	
	Resource use, energy carriers	2	

- Workflow relevant to Step 4
- The scheme refers to steps to be followed to assess environmental sustainability and is not entailing exclusion criteria

Step 5 - Scientific basis for the socio-economic sustainability assessment

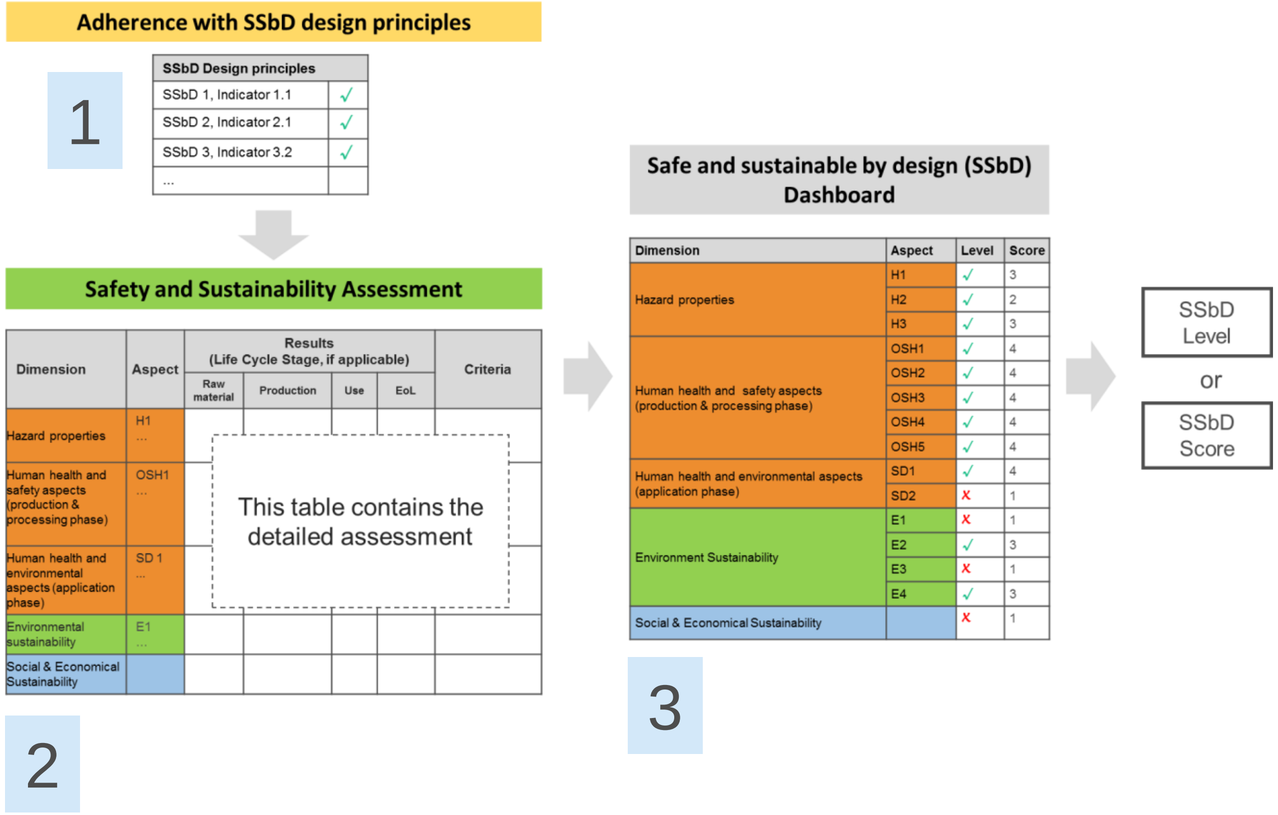
- This step explores available approaches for the Social and Economic Sustainability assessment.
- In the case of **social assessment**, it describes which are the relevant stakeholders and social aspects that could be used for the social assessment.
- The **economic assessment** part focuses on non-financial aspects, e.g. the identification and monetisation of externalities arising during the life cycle of a chemical or a material.
- These aspects are included in the framework to be explored as methods still need to be further developed.
- Given the limited level of its implementation, further work is needed in order to ensure applicability in the framework for SSbD chemicals and materials.

Evaluation procedure

Overview of the evaluation components

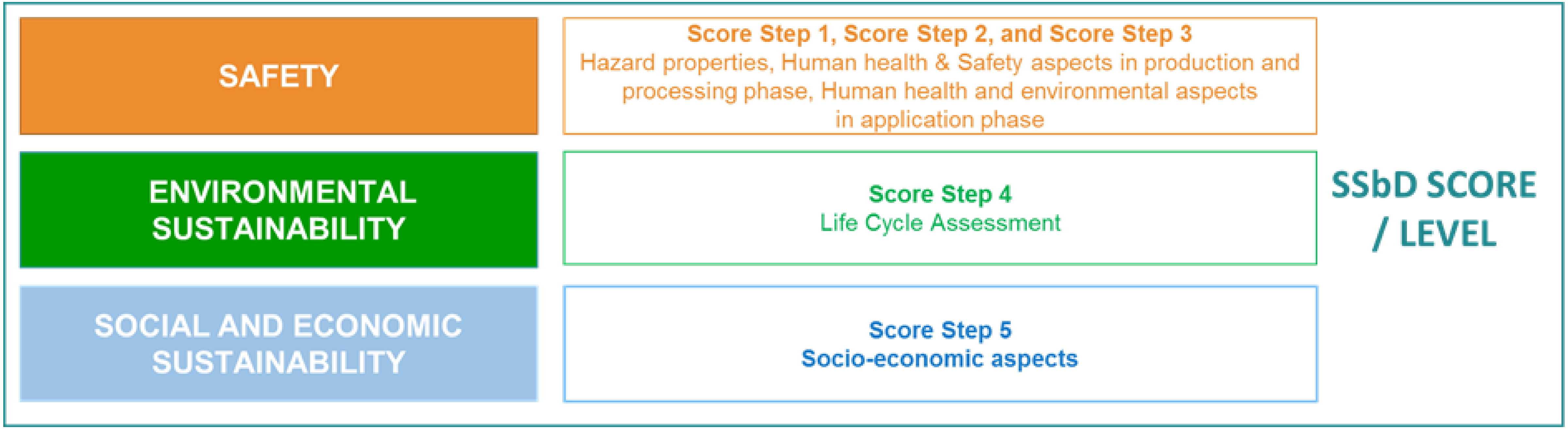
The application of the framework will provide three outputs:

1. The adherence to the SSbD principles during the design phase;
2. The safety and sustainability assessment, namely the detailed figures on the performance of the chemical/material against the SSbD criteria;
3. A dashboard summarising the results of the safety and sustainability assessment is proposed as a tool to facilitate informed conclusions/decisions based on a holistic assessment.



Evaluation procedure

Overall evaluation procedure combining the assessment results of all dimensions



Data availability and uncertainty

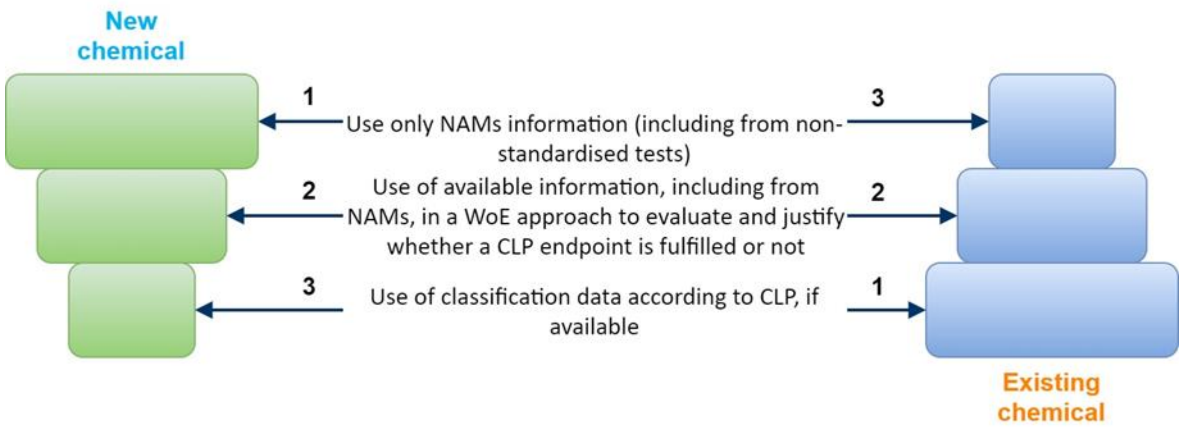
Data sources

- In order to perform the assessments described in the framework, each step will require reliable data sources and tools that can process the information
- The assessment steps refer already to some specific tools that can be used for the case studies demonstration.
- As a starting point and in addition to the tools already mentioned in the description of the Steps 1-3, sources such as ECHA's Information on Chemicals , EFSA' Chemical Hazards Database (OpenFoodTox) , OECD’s eChemPortal , EPA's CompTox, can be used.
- Data availability can also be a challenge for conducting the LCA in as proposed in Step 4. An example of available databases for Environmental Footprint LCI datasets is available on the European Platform for Life Cycle Assessment.
- Additional examples of data sources were included in *Caldeira et al., 2022, https://data.europa.eu/doi/10.2760/879069 (review)*

New Approach Methodologies (NAMs) in the context of SSbD framework

- In the context of SSbD framework, NAMs and data generated using non-animal methods are of utmost importance for the safety assessments
- SSbD framework should be seen as a tool to support and promote NAMs use and at the same time, SSbD concept should be a beneficiary of the developments in this area
- NAMs are important to guide the process of developing new substances as they are likely to be helpful at early stages in the substance development process

*A **tiered approach** regarding the information requirements, to be applied depending on whether a new or an existing chemical is evaluated - to allow the assessment to be performed already at an early stage of the innovation process and use all available information, including from NAMs*



*"Safety testing and chemical risk assessment need to innovate in order to <u>reduce dependency on animal testing</u> but also to improve the quality, efficiency and speed of chemical hazard and risk assessments" **EU Chemicals Strategy for Sustainability***

***NAMs** = various approaches for generating data by using non-animal methods and technologies; use of individual non-animal methods, such as in vitro methods, as well as in chemico or in silico methods (e.g. QSARs), the use of combined and stepwise approaches, such as integrated testing strategies (ITS) or integrated approaches to testing and assessment (IATA) (ECHA, 2017; EC JRC, 2021)*

Data quality and uncertainty

- Data quality and uncertainty is a concern for the different aspects assessed in this framework that needs to be addressed
- Additional data quality criteria as well as minimum data (information) requirements need to be defined and implemented to complement the SSbD criteria, ensuring that relevant and high-quality data is used for the sustainability assessment.
- Several approaches exists (e.g. ISO, Pedigree Matrix concept, EU JRC’s ILCD and Environmental Footprint methods, GreenScreen) and are evaluated for further adaptation to the framework specificity
- A general requirement for data sources used for the SSbD assessment is that they provide data in a findable, accessible, interoperable and reusable (FAIR) format.

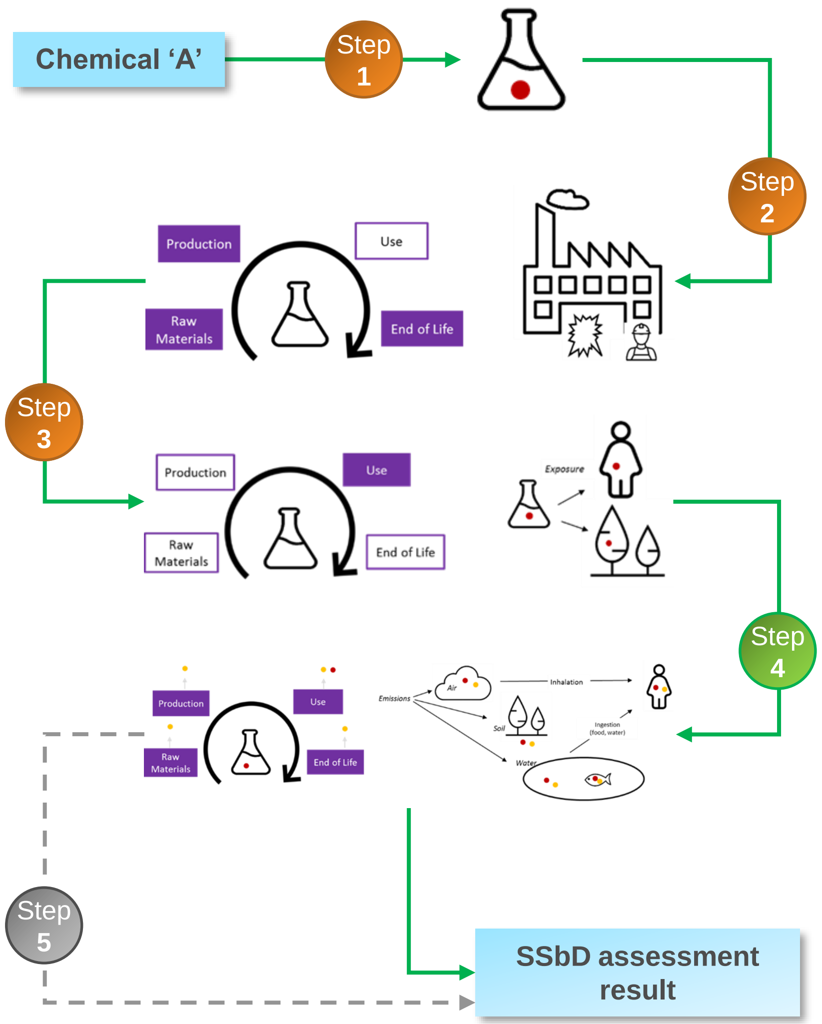
Next steps

Testing phase and case studies

- Three case studies are considered in order to:
  - Assess the SSbD methodology and its feasibility
  - Identify the data needs and availability
  - Define specific criteria
  - Provide additional knowledge for the optimisation and refinement of the methodology

- 3rd JRC Technical Report on the elaboration of criteria with application to one case study (expected Q2 2023)
  - Consultation with stakeholders (3rd Stakeholder workshop to be organised in Q1 2023)

SSbD assessment workflow



Selection of chemicals or materials

- Examples of case studies

Group	Application	Description
Plasticisers (*non-phthalate*)	Food contact materials (FCM)	Case study on phthalate-free plasticisers, as an example addressing consumer exposure
Surfactants	Textiles processing	Case study on surfactants used in the textile processing during the cleaning phase (scouring)
Flame retardants (*halogen-free*)	Information and communications technology (ICT) products	Case study on flame halogen-free flame retardants, addressing circularity and also consumer exposure

- Selection based on the input received in the stakeholder survey (June 2021) and alignment with relevant EC policies
- Analysis of information on these possible case studies and evaluate the relevancy in the context of the SSbD framework:
  - Identification and description of chemicals belonging to these groups
  - Alternatives available
  - Data availability

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Thank you

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