SAFE AND SUSTAINABLE-BY-DESIGN:
A GUIDANCE TO UNLEASH THE TRANSFORMATIVE POWER OF INNOVATION

MARCH 2024

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Foreward

The chemical industry is a vital player in Europe's economy, driving innovation and thereby competitiveness not only for the chemical industry, but also for the many value chains it operates in. Today, the European chemical industry is at a crossroads. We support the goals of the European Green Deal and Europe's ambition to become climate neutral by 2050. Yet, implementing the Green Deal agenda represents a so-called 'double twin' transition for our sector. We need to become climate neutral, circular, innovate towards safe and sustainable chemicals, and digitalise our industry. And we must do it all while remaining competitive in the global market to keep a thriving chemical industry in Europe. This requires a massive effort from our industry and all connected value chains.

With this in mind I am proud to introduce our new guidance on how to innovate and design with safety and sustainability in mind. This concept, which we view as a holistic approach, integrates Safe and Sustainable-by-Design (SSbD) principles from the very start of the innovation process. This ensures that innovative products and processes show improvements in their respective performance and in the area of safety and sustainability. The guidance serves as an important tool that supports companies in understanding, testing, and implementing SSbD principles. It is a clear indication of our commitment to advancing a sustainable future.

We view SSbD principles as foundational, aligning with the broader goals of the European Green Deal and the Chemicals Strategy for Sustainability. As an example, Cefic's Long Range-Research Initiative (LRI) has, over the past 25 years therefore long before SSbD frameworks were discussed, supported multiple projects for the development of tools that are already widely used and accepted in the field, and hence now are seen as highly relevant for the development of an SSbD assessment toolbox.

In applying SSbD principles, the chemical industry aims for a continuous science-based reduction of toxicological risks for humans and the environment, especially for consumer use, while also considering end-of- life and circularity aspects. Our efforts to test and further develop the guidance reflect a proactive approach to meeting the challenges, marking a significant step in our journey towards sustainability.

This guidance aims to offer a balanced perspective, acknowledging both industry's views and other positions in the field, as outlined by entities like the European Commission, the Joint Research Centre (JRC), the Organisation for Economic Co-operation and Development (OECD), and the World Business Council for Sustainable Development (WBCSD). Our goal is to foster a dialogue, clarifying the industry's aspirations and policy expectations. This effort seeks to constructively interact and promote a shared understanding that benefits all stakeholders.

This guidance report marks a milestone in our journey towards integrating Safe and Sustainable-by-Design (SSbD) principles more deeply within innovation processed in the chemical industry. It emphasizes our commitment to a dynamic process of testing and refining the proposed SSbD guidance, with companies now testing its application. This effort ensures that the SSbD guidance is practical, aligned with the sector's needs while having the envisioned impact. This testing might lead to further framework developments as our experience with the application of the framework grows. At Cefic we are dedicated to guiding our members through this process, offering expertise to facilitate the transition towards safer and more sustainable practices.

We invite all stakeholders to join us in this collective initiative, aiming for a chemical industry in the EU that is safe, sustainable, innovative, and competitive.

This guidance is an outcome of the collaborative efforts and insightful exchanges among the Cefic members in the SSbD Network of Experts. I extend my sincere gratitude to the dedicated writing team.

I hope you get inspired by our guidance report and join us in this exciting journey!

Sincerely yours,

Daniel Witthaut, Cefic Executive-Director for Innovation

Table of content

Preamble 5

Executive Summary 6

1. The transformative power of Innovation based on Safe and Sustainable-by-Design principles 7

1.1 Background 7

1.2 Safe and Sustainable-by-Design: guiding the innovation process 8

1.3 Identifying innovation needs using a Product Sustainability Assessment Framework 10

1.4 Transparency and non-financial reporting 11

2. Safe and Sustainable-by-Design in practice 12

2.1 The innovation process 12

2.2 The "safe" and "sustainable" assessment framework 13

2.3 Incorporating Safe and Sustainable-by-Design into the innovation process 14

2.3.1 Idea Creation - going from Gate 1 to Gate 2 16

2.3.2 Feasibility Study - going from Gate 2 to Gate 3 16

2.3.3 Laboratory or Development Phase - going from Gate 3 to Gate 4 16

2.3.4 Scale-Up & process development - going from Gate 4 to Gate 5 17

2.3.5 Launch 17

2.4 Safe and Sustainable-by-Design in action 17

2.4.1 Define performance and functionality needs – Activity 1 17

2.4.2 Assessment Dimensions – Activity 2 17

2.4.3 Design Principles – Activity 3 20

2.4.4 Comparative assessment – Activity 4 24

2.4.5 Trade-offs – Activity 5 32

3. Conclusion 34

3.1 Concluding remarks 34

3.2 Connect the PSA assessment framework with the assessment dimensions of an SSbD approach 34

4. Needs and next steps 35

Annex 1 – Definitions 36

Annex 2 – Authoritative and other relevant substances lists 37

Notes 38

Preamble

A guidance on Safe and Sustainable-by-Design

Cefic and its members have defined Safe and Sustainable-by-Design (SSbD) as an iterative process guiding innovation and the placement on the market of new chemicals, materials, products, processes and services that are safe, and deliver environmental, societal, and/or economical value through their applications. Subject of the document are new chemicals, materials, products, processes and services, as well as potentially re-designing existing ones identified through portfolio analysis (see below Portfolio Sustainability Analysis).

Scope

To identify relevant dimensions for safety and sustainability, we could rely on the experience of chemical companies implementing the framework for Portfolio Sustainability Assessment, developed and kept up to date by pioneering companies under the umbrella of the WBCSD[1]. In this methodology for the chemical industry, the following "signals" need to be assessed e.g., the chemical hazards and exposure across the life cycle, anticipated regulatory trends, sustainability ambitions along the value chain, authoritative ecolabels, sustainability related certification and standards, environmental and social performance across the life cycle compared to alternative solutions. Other "signals" are recommended to be assessed, the sustainable value creation, the Sustainable Development Goals[2] and the company's internal guidelines & objectives.

The application scope that the writers of this guidance have in mind is research and innovation for safe and sustainable chemicals as put forward in the Chemicals Strategy for Sustainability (CSS)[3]. The innovation goal of the CSS is said specifically to bring solutions across sector markets, notably for construction materials, textiles, low-carbon mobility, batteries, wind turbines and renewable energy sources. For the European chemical industry this translates to innovation challenges on how to design for safe and sustainable chemicals, materials, processes & services linked to these market segments. These innovations can be breakthrough (e.g. Advanced Materials) or incremental (following an improvement process) regarding the safety and sustainability attributes. In this version of the guidance, the socio-economic assessment has not been covered.

Target Audience

This guidance is intended to be used on a voluntary basis by Research & Innovation teams within chemical companies and is offered as complementary of information for the ongoing work at the European Commission regarding the developments of a framework for Safe and Sustainable-by-Design components.

Whilst this guidance is addressing in the first place Cefic members, we'd consider it good practice to extend its use to international value chains and other parties involved in Research and Innovation within the chemical and further sectors where the guidance has relevance as well.

Requirements for Success

The European chemical sector has the ambition to deploy safe and sustainable solutions to make the transition towards a climate-neutral, circular and so-called "toxic-free" society possible. With this guidance, we want to contribute to the exciting transition journey by giving input to the ongoing framework developments initiated by the European Commission, supported by the Joint Research Center[4]. We see this Cefic guidance as an example of how industry can implement Safe and Sustainable-by-Design principles into the innovation process in a practicable, workable way forward.

The sector further commits to continue innovating for assessment methodologies, as it has done for the last 25 years through e.g. Cefic's Long-Range Research Initiative (LRI), and to obtain and transparently share the knowledge supporting the assessment methodologies. In doing so, we in particular seek to also support those industry members that due to their workforce size do not have all kinds of diverse expertise needed to perform a SSbD assessment in house as foreseen by e.g. the JRC framework in its current state. In addition, we also want to ensure consistency with larger companies.

The so-called Green transition sets an unprecedented challenge for the chemical industry, Safe and Sustainable-by-Design principles outline a way forward. It will be important to flank this transition vision with enabling policy measures to ensure predictability of goals, within timelines that are ambitious yet realistic. Providing for the skills and resources – financial and non-financial – needed, is a prerequisite.

We believe, a thorough co-development of the concept and its implementation, involving all relevant stakeholders, will result in a powerful and effective approach towards safe and sustainable products, strengthen the European industry's competitiveness and lead to increased supply and production security within the European Union.

We are committed to spread this guidance, to support industry in testing it's applicability to the entire panorama of companies operating in different sectors, and report on its application in a transparent and validated way.

Executive Summary

Cefic and its members have defined, in their previous reports from October 2021 and April 2022, Safe and Sustainable-by-Design (SSbD) as an iterative process guiding innovation and the placement on the market of solutions that are safe, and deliver environmental, societal, and economical value through their applications. In scope are new chemicals, materials, products, processes and services, as well as the potential re-design of existing ones, e.g. identified through Portfolio Sustainability Analysis (WBCSD).

Based on Cefic's previous work, this report proposes **guiding design principles** for a selected set of safety and sustainability considerations or **dimensions** to be assessed at the level of product-application combination in a stage-gate-like approach during innovation.

Identifying the relevant assessment dimensions early in the process, and subsequently setting guiding design principles for the most important dimensions, will increase the speed and likelihood to bring solutions to the market (fail fast – fail cheap).

The **basic principle** when innovating to improve the functionality and performance of chemicals, materials, products, processes or services, is the aim to **improve** performance in at least one of the dimensions of safety and sustainability without significant negative impacts[5] in any of the other dimensions, compared to the incumbent solutions.

As a minimum, a sound implementation of **"Safety"** shall be applied by a risk-based assessment considering the hazard, use and exposure in line with REACH and anticipating future regulatory changes. But in applying SSbD, the chemical industry has the ambition to go beyond that legally fixed requirement and go for continuous reduction of toxicological risks for humans and the environment especially for consumer use and considering end-of-life and circularity aspects. The assessment relies on efficient comparative screenings in early stages and as a result, assessment tools, information and criteria need to evolve over time. We have illustrated this approach with practical examples.

The **"Sustainability"** assessment[6] as an integral part of the innovation process shall cover the life cycle of a product-application-combination. All assessments shall, as a minimum, cover focus dimensions deemed of high importance to reach the Green Deal objectives. Additional sustainability contributions may be considered.

Finally, selecting candidates or making choices on alternatives is an activity that runs through almost all stages of the innovation process. Seldom will a solution present itself outstanding in all the relevant assessment dimensions for an intended product-application. Choosing between candidates and making trade-off decisions are indeed more the rule, than the exception. That's why this guidance also spends some thoughts on trade-off practices.

In conclusion, for SSbD to become a useful guidance for fast decision making in (industrial) innovation processes, approaches must be:

- lean and pragmatic
- resource and capacity needs should be coverable by the respective existing innovation project resources.

As it can be seen by the previous, bringing in safety and sustainability considerations early into innovation processes is relying heavily on data and assessment methodologies. Hence, the development of further flexible, adaptable (digital, e.g. predictive approaches such as modelling) methodologies and toolboxes including withgoing databases, will be needed; the same is applicable for investments and additional incentives to strengthen the global competitiveness of the EU chemical industry.

And finally, Cefic continues to support the co-creation of a straightforward and implementable approach to Safe and Sustainable-by-Design innovation between the European Commission, industry, academia and RTOs and the downstream users of the chemical sector. Cefic commits to continuing the facilitation of this co-creation process, bringing together all relevant stakeholders.

1. The transformative power of Innovation based on Safe and Sustainable-by-Design principles

1.1 Background

On October 14, 2020, the European Commission published the Chemicals Strategy for Sustainability (CSS)[7] as part of the European Green Deal's pillar[8] "Zero Pollution Ambition[9]". The Green Deal, the main policy initiative of the Von der Leyen Commission, aims to achieve a climate-neutral, pollution-free, sustainable, circular and inclusive economy by 2050.

The goal of the CSS is to guide the green transition of the chemical sector and its connected value chains. Aligned herewith are the goals of the New Industrial Strategy[10] for Europe promoting a green and digital transformation of the European industry in general.

The capacity of manufacturing new chemicals that are "inherently safe and more sustainable from production to end-of-life[11]" including circularity considerations is said to play a crucial role in the green and digital transition. Chemicals and materials from a Safe and Sustainable-by-Design (SSbD) R&I approach[12] will be promoted on the EU market, with the strong ambition to become a worldwide standard in the future. One closely linked vehicle to steer the development of new products, and therewith also chemicals, towards "inherently safe and more sustainable" is the Ecodesign for Sustainable Products Regulation (ESPR)[13] which is currently under development. There, on a product group basis, requirements on the use and information sharing e.g., for certain chemicals will be implemented. As a carrier for such information the Digital Product Passport (DPP) will be introduced.

Through its up-stream positioning, the chemical industry has a significant impact on almost all value chains with >90% of all manufactured goods depending on chemicals, resulting in a key pivotal and enabling position to realise the European Green Deal ambitions. To foster this transition, the EU is taking a dual approach of restricting and banning existing hazardous substances in certain applications, and fostering innovation for new safe and more sustainable chemical products by respectively:

1. putting in place a more preventive (or stricter) approach to regulate the use of the most harmful chemicals, especially in consumer goods;
2. development and implementation of a pre-market Safe and Sustainable-by-Design approach for new, innovate solutions for the development of new chemical products and the potential re-design of existing ones, following a Portfolio Sustainability Analysis;

On SSbD, the European Commission recently (December 8, 2022) published a *Recommendation on the establishment of a European assessment framework for "Safe and Sustainable-by-Design" chemicals and materials*[14]. Prior to this recommendation, in October 2022, the Commission's Strategic Research and Innovation Plan (SRIP) for safe and sustainable Chemicals and Materials was presented to the public[15]. Within these documents, the CSS and in alignment with the Green Deal objectives, three overarching goals for the development of SSbD products become evident: i) protection of humans and the environment from the "most harmful chemicals[16]" ii) enabling circularity, and iii) contribution to resource efficiency. These goals should be considered by all innovators, from the innovation phase towards the development of products.

Cefic has presented its preliminary views on SSbD, and how to take it forward in two previous reports, that were both made available to the public before the European Commission published both the SRIP and the Recommendation on the SSbD framework[17]. In this paper, we are presenting additional views with more concrete, hands-on guidance on how to integrate considerations on safe and sustainable solutions into the research & innovation process. The guidance is based on distinctive activities to be taken at different stages of industrial research & innovation processes. It also reflects crucial points to be addressed such as differences in e.g. data availability depending on the maturity level of innovations, the paramount importance of having a clear use case in mind (product-application connection), a discussion around trade-off decision making and how to practically address those.

1.2 Safe and Sustainable-by-Design: guiding the innovation process

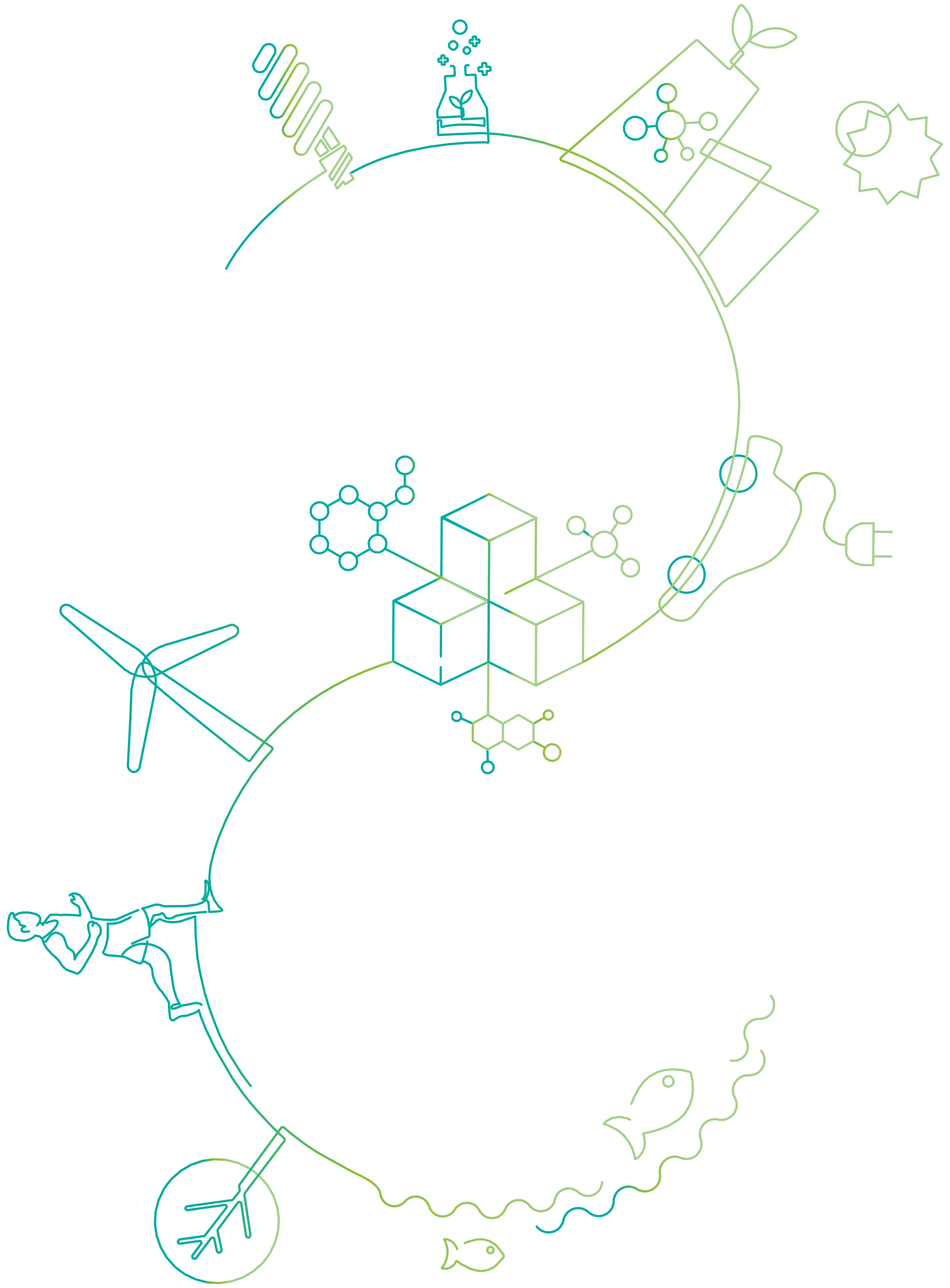
Safe and Sustainable-by-Design is an iterative process guiding innovation and the placement on the market of solutions that are:

- safe, and
- deliver environmental, societal, and economical value through their applications.

Hence, the SSbD process should enable the design of **the next generation chemicals, products, processes and services** for a resilient economy, including transitioning to a climate neutral society, circular economy and avoiding harm to people and planet.

We propose the SSbD concept to be implemented as a **process** based on **guiding design principles** for the Research & Innovation phase of all new products using dimensions to be assessed at the level of product-application combination in a stage-gate like approach during innovation.

- The basic principle when innovating to improve the functionality and performance, is the aim to improve performance in at least one of the dimensions of **safety and sustainability** (Figure 8 and Figure 9) without significant negative impacts[18] in any of the other dimensions (e.g. performance applications, acceptable cost...), compared to the incumbent solutions.
- As a minimum, a sound implementation of "Safety" shall be guaranteed by a risk-based assessment considering the hazard, use and exposure in line with REACH and anticipating future regulatory changes. In applying SSbD, the chemical industry has the ambition to go beyond that legally fixed requirement and to commit to advance scientific progress towards ever more knowledge in the field of toxicological risks for humans, and the environment, especially for consumer use and considering end-of-life and circularity needs.
- The sustainability assessment[19] as an integral part of the innovation process shall cover the life cycle of a product-application-combination. All assessments shall, as a minimum, cover focus dimensions deemed of high importance to reach the United Nations Sustainable Development Goals and Green Deal objectives. Additional sustainability contributions (environmental, societal and economic) may be considered. A comprehensive, yet not exhaustive list of safety and sustainability dimensions typically proposed by different stakeholders for consideration when assessing sustainability aspects is presented schematically below (Figure 1) and further detailed in paragraph 2.4.2.3



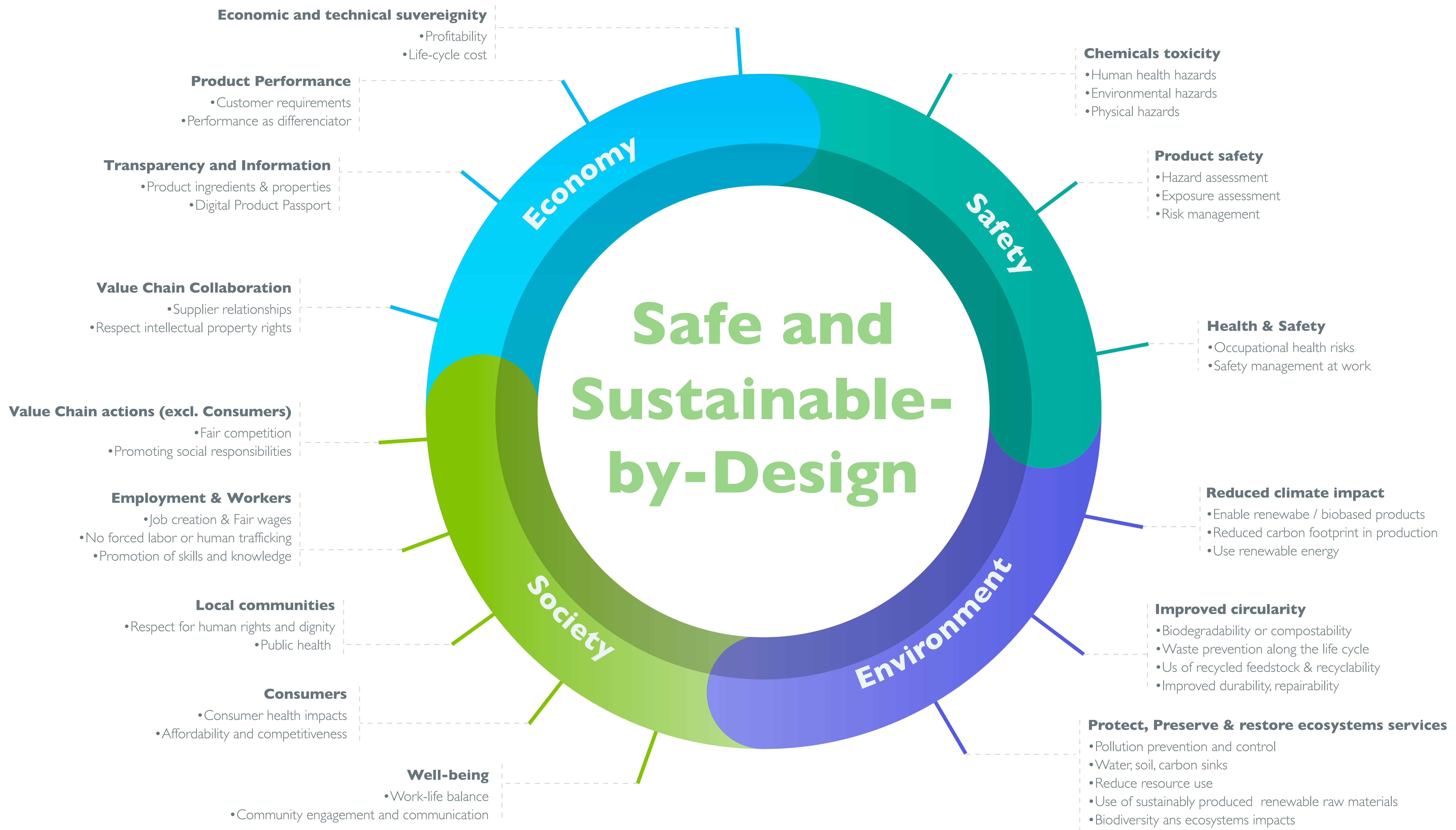


Figure 1: A comprehensive, yet not exhaustive list of safety and sustainability dimensions to assess and design sustainable chemicals, materials, products and processes.

1.3 Identifying innovation needs using a Product Sustainability Assessment Framework

Given that chemicals are part and parcel of over 90% of manufactured goods, the chemical industry has an impact on almost all value chains, and is therefore a key player in enabling the ambitions of the EU Green Deal. To innovate towards tangible improvements with regards to "safe" and "sustainable", it is of great importance to always consider the full life cycle of a chemical product in its respective application. The development stage, production, use phase and end-of-life should be considered with regards to their specific requirements.

For an efficient and effective transformation of the product portfolio, the Safe and Sustainable-by-Design framework should be applied to all new chemicals, material, product, process and service innovations. Innovation should be interpreted broadly, also covering minor changes e.g., potential re-formulations. In the case of minor changes, a simplified check can be used for the assessment. In doing so, the approach, over time, will thus "influence" the composition of the full product portfolio.

Assessing regulatory and other signals covering chemicals safety and sustainability, as promoted in the Portfolio Sustainability Assessment[5] (PSA) methodology including its recent update[20] is an established practice already in more than 20 chemical companies[21] around the globe.

The assessment results of the existing portfolio, based on product-application combinations, are clustered in so-called sustainability performance categories and then aggregated on portfolio level based on the products' sales contribution:

Consequent prioritisation of industry sectors, e.g., fast moving consumer goods, but also market signals, including regulatory follow-up,

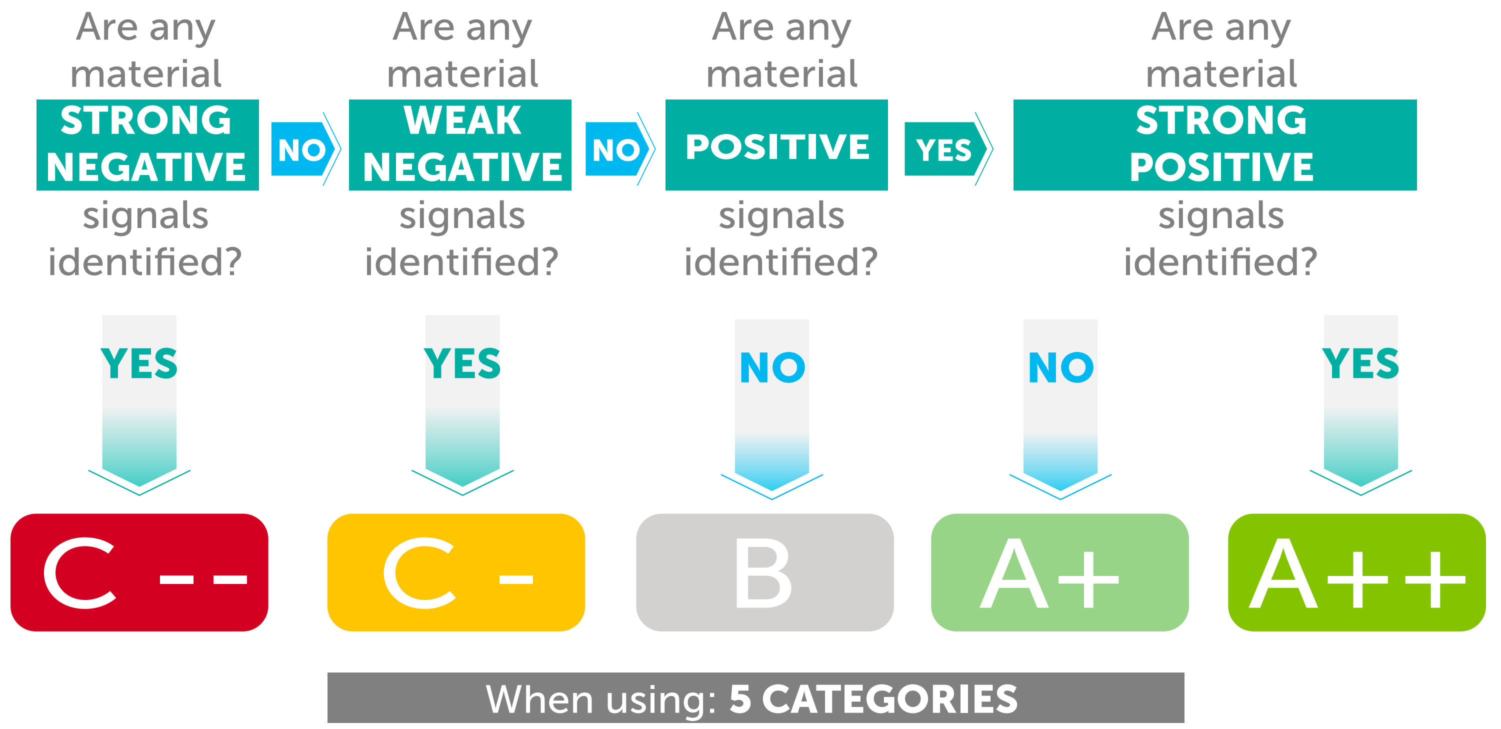


Figure 2. WBCSD Decision tree towards sustainability performance categories on a "Product-Application-Region-Combination" (PARC) basis (in this example 5 categories).

will help companies to leverage the biggest impacts first. Implementing the generic framework of the PSA 2.0 methodology by the WBCSD can thus help identify the company's innovation needs. Linking the Safe and Sustainable-by-Design concept as an innovation approach to the PSA framework will bring up safer and more sustainable products in the sense of a continual improvement process.

Coupling the assessment and ranking of the portfolio with the company's innovation process will in a continuous journey over time move the portfolio of products towards ever safer & more sustainable chemicals, materials, products and processes in the context of their specific life cycle.

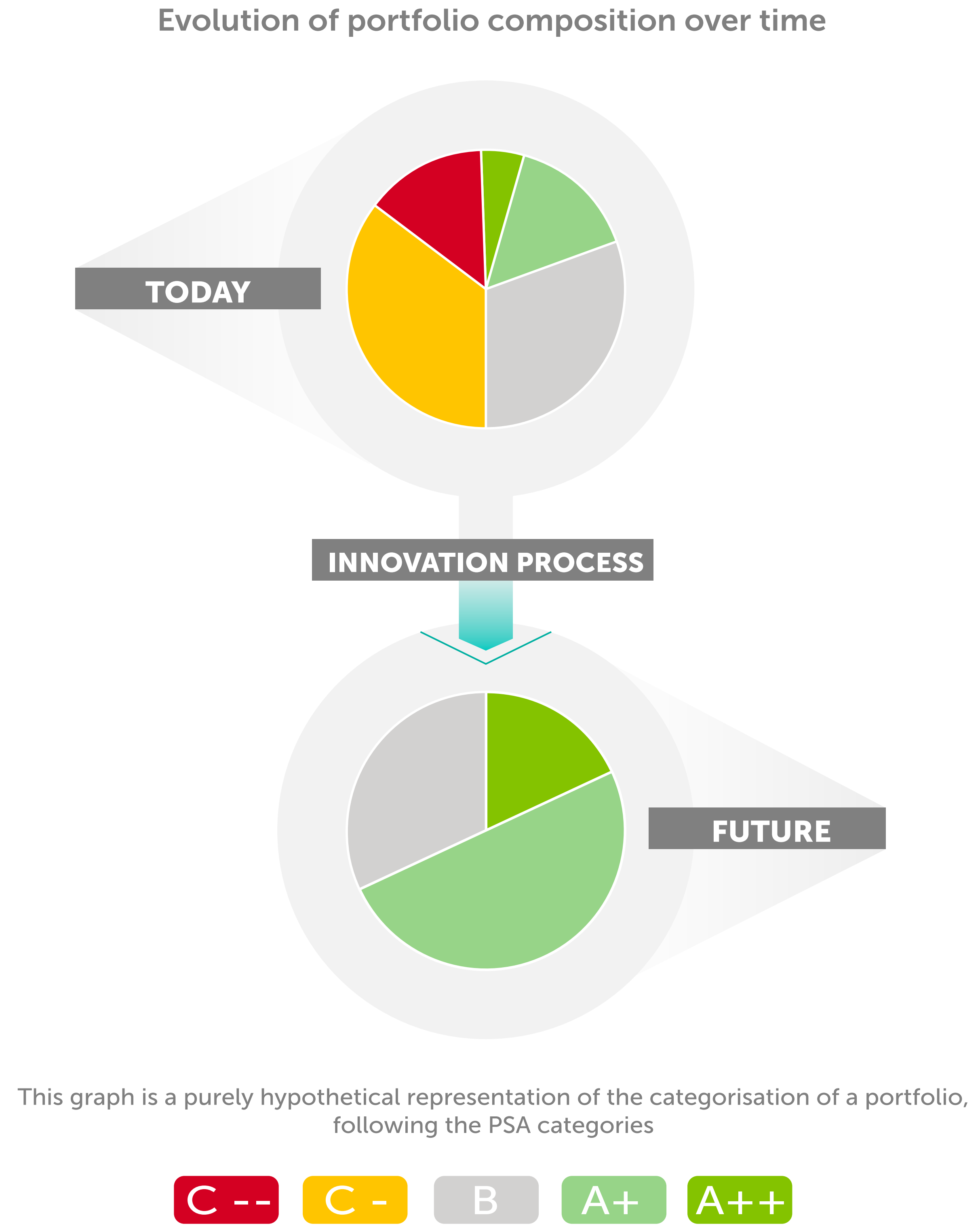


Figure 3. Schematic depiction, how applying the SSbD principles over time will move the portfolio of products towards safe & sustainable chemicals, products and processes.

1.4 Transparency and non-financial reporting

Sustainability needs transparency and transparency should ensure comparability in assessment methodologies through harmonised terminology and standards. At the same time, the assessment methodology needs to take into account the different stages of the design process, as well as the differences in innovations e.g., between improvement of existing products to the design of totally new products.

Data required supporting the respective assessment need to be FAIR (findable, accessible, interoperable and reusable). Special attention for the needs of SMEs on tools and supporting data will be necessary.

Companies are advised to report on their journey towards enhanced safety and increased product sustainability. For instance, using harmonised standards for Product Carbon Footprint (PCF) calculation such as ISO 14040, ISO 14044 and ISO 14067 and reporting in line with the Together for Sustainability (TfS) guidelines increase comparability. Furthermore, reporting on the companies' PSA improvements which contributes to ESG achievements is considered good practice.

2. Safe and Sustainable-by-Design in practice

Industry views the application of SSbD principles as a pre-market concept to ensure innovation towards future enhanced safety and increased product sustainability. Reflecting the huge variety of consumer products and services, it is recommended to conduct Safe and Sustainable-by-Design assessments on **a product-application level** with the **intended use** and the level of improvement targeted (depending on the market and the current "state of the art") in mind.

2.1 The innovation process

Most companies innovating in the chemicals industry today employ a staged or phased process to guide the research on and development of new innovations from idea to market launch. Typically, such a staged management process is used to assist in decision making whether to continue development work as more information becomes available. The process has been made popular by Robert G. Cooper as the Stage-Gate™ process[22]. Companies mostly will consider a 5-stage process with some form of Go/No-Go decision point between each stage ("gate"). Many variations exist - here we will refer to a general case.

The process starts with the **ideation**, generating ideas to create options in the form of new opportunities or problems connected to a particular product-application combination to be solved as well as opportunities in new technology fields that might be capitalised on. At this stage, the overarching innovation goal for performance and functionality are being identified. The next step is the **conceptualisation**, to create alternative options to understand and define a problem, an opportunity or new technology field as well as envisioning concepts that help to solve it. After business planning, experimental work in the **laboratory** follows, where the different concept candidates are tested and evaluated against the targeted innovation goals. With ongoing **validation**, the number of suitable candidates decreases. If one of the candidates fulfils all innovation goals (functionality, safety, sustainability, economy), the candidate will proceed to the **launch phase** and be placed on the market. If no candidate matches all innovation goals, it will be important to identify the best suited candidate which will often involve trade-off decision making (See chapter 2.4.5). Before getting to this final stage, the research & innovation process often loops back-and-forth between earlier steps (iterative steps), affecting predictability of duration and overall success of project quite significantly. A general simplified depiction of the Stage Gate process is given in Figure 4.

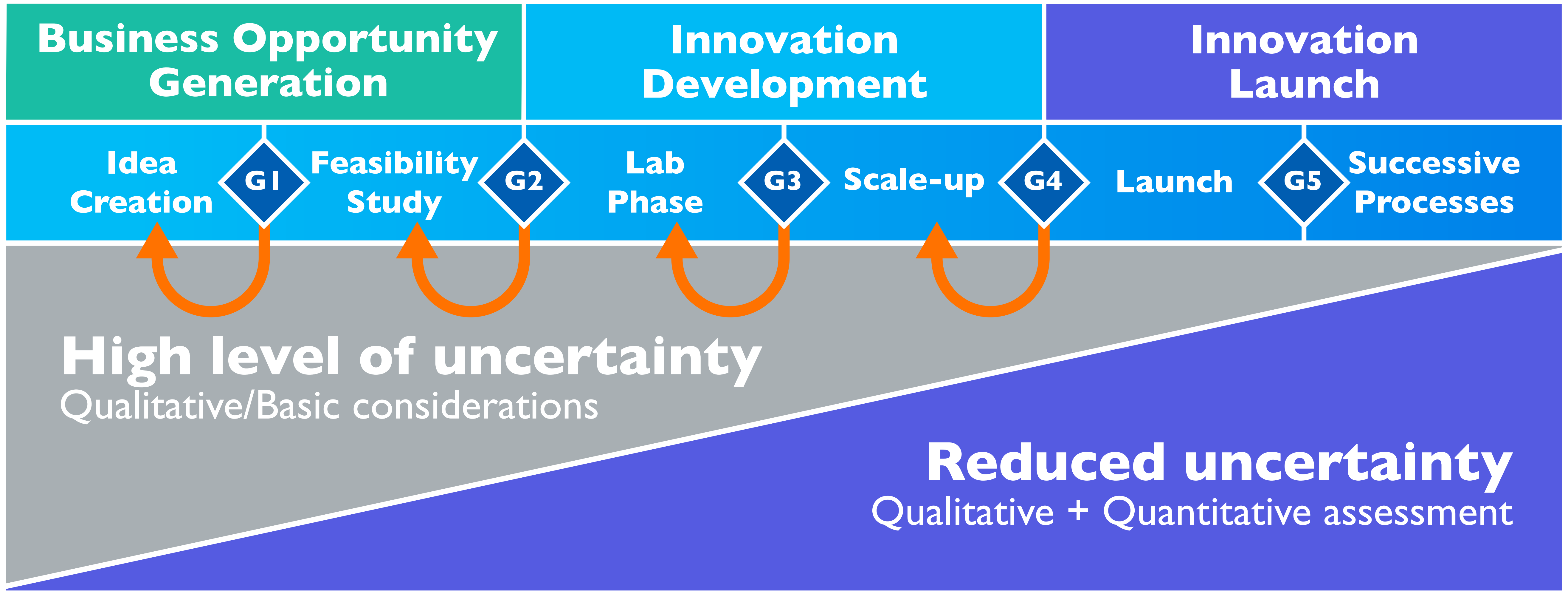


Figure 4. Simplified and idealised depiction of an iterative innovation process illustrating the increasing level of available detail for the safety and sustainability evaluation of new products

2.2 The "safe" and "sustainable" assessment framework

In line with the needs of a generic innovation process as depicted under 2.1, the assessment guidance is proposed as a layered structure to foster Safe and Sustainable-by-Design developments as envisaged along five activities (Figure 6, activity 5 - trade-off decision making - not shown, as this is an overarching constant activity to be considered in conjunction with all other activities). Out of these, activities one to three are interdependent and should be carried out in parallel as they define the scope of the assessment (activity1 – 2.3.1). These activities support the identification of performance and functionality needs related to a specific, pre-defined use case of the envisaged innovation, including considerations for safety and sustainability. The definition of the use case is of utmost importance for determination of the exposure scenarios. It has to be noted, that a differentiation is made between industrial/production process use and the consumer use phase, incl. professional use in addition to end-of-life considerations.

As a consequence, relevant dimensions can be identified material for the assessment under the key words "Safe" and "Sustainable". These dimensions can be adopted in a modular fashion in activity 2 (chapter 2.3.2) subject to the use case definition. The identified dimensions indicate which aspects to look into in the innovation's ideation phase that need to be further assessed prior to launching a solution, covering the full life cycle. Within the dimensions, we differentiate between focus dimensions and additional dimensions:

- **Focus dimensions** are deemed to be critical to meet the EU Green Deal goals and should always be assessed

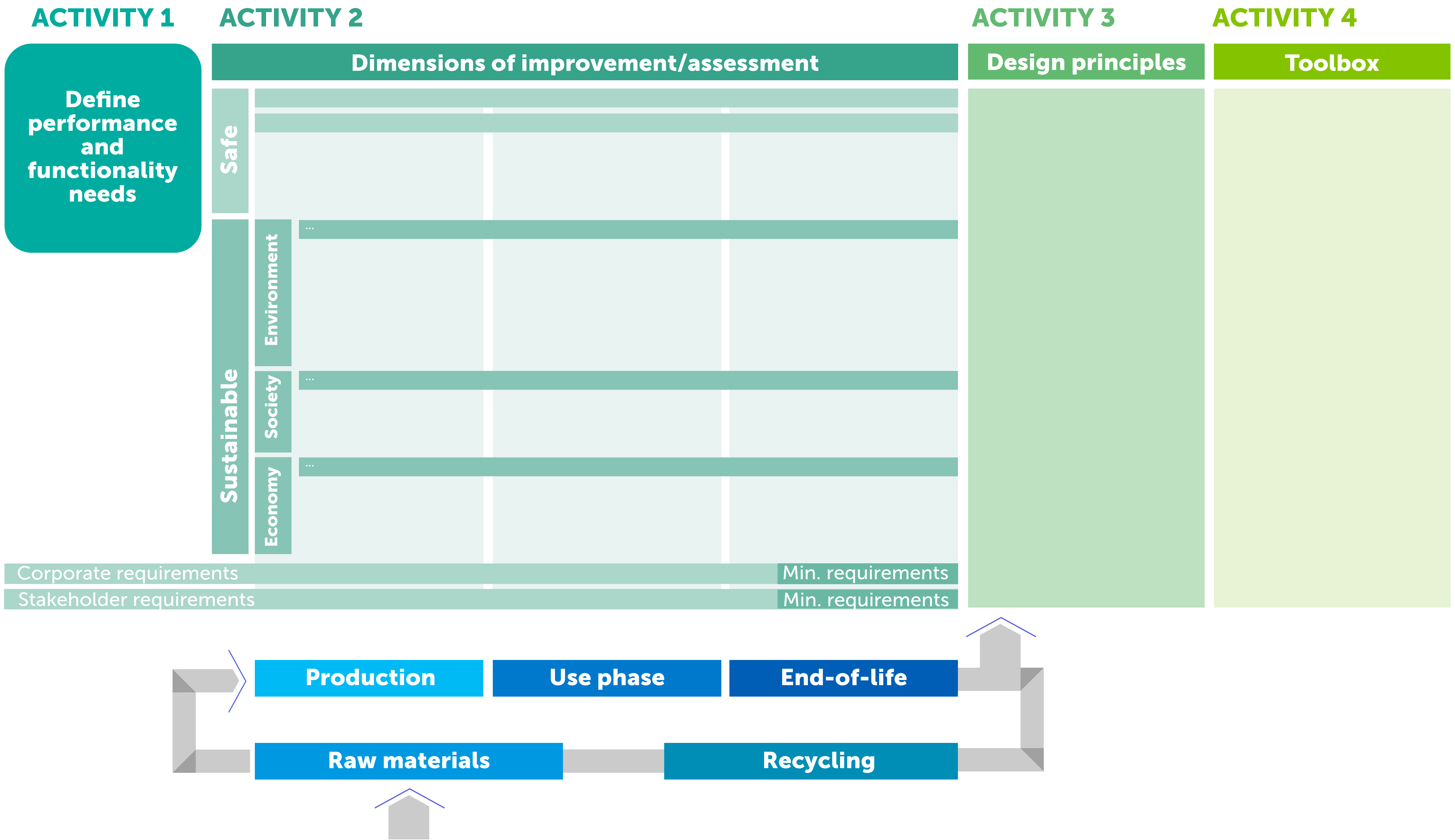


Figure 5. Overarching depiction of the Safe and Sustainable Assessment framework as proposed in this report
Note: depiction of activity 5 - trade-off decision making - is missing, as this is a constantly ongoing activity in conjunction with all other activities.

- Additional dimensions are any other dimension that should be assessed if identified as material for the intended use case.

Next, we identify **minimum requirements** to be fulfilled at all times, e.g. respecting human rights and complying with the regulatory requirements as defined in applicable law.

The focus dimensions are associated with **design principles** to be considered as guidance, which are to be selected in activity 3 (chapter 2.3.2) in conjunction with the defined use case. The principles give hands-on guidance on which aspects should be considered when designing a chemical, material, product, process, or service, raising the level of awareness for the search of optimization potential in the respective dimension.

Activity 4 and 5, which in turn are interdependent with activities 1-3 (See chapter 2.3) support the decision taking in a stage gate assessment approach between several innovation candidates from the lab to launch phase, also guiding through potential trade-offs. Suggestions how to set-up and conduct the comparative assessment are described under activity 4 (chapter 2.3.4). Starting with the differentiation of must-have and good-to-have requirements, a robust screening/testing strategy for the envisaged innovation should be derived utilizing meaningful tools/indicators. Based on those indicators informed decision taking should be enabled and FAIR data (FAIR: findable, accessible, interoperable, and reusable) should be generated. This allows for a specific safety and sustainability assessment depending on the current stage of an innovation.

Along the decision taking at any stage in the innovation process, trade-offs will need to be made. Guidance as how to handle those, trying to prevent regrettable substitution and aiming at the best optimization iteration possible, can be found in activity 5 (chapter 2.3.5).

A depiction of the assessment framework structure can be found in Figure 5. A practical description of the safety and sustainability assessment can be found in chapter 2.3.

2.3 Incorporating Safe and Sustainable-by-Design into the innovation process

Any framework for the development of new safe and sustainable chemicals, materials, products and services, will require a flexible structure accounting for the vast variety in chemical products going into several applications, resulting in multiple combinations of sustainability assessments including hazard and exposure along multiple life cycle paths. In addition to this structure, the framework also needs to consider the high level of uncertainty due to limited information availability, especially at early innovation stages. Information on product properties, performance level and consequently also on safety and sustainability of the product might lack at the beginning of an innovation process, especially where completely new chemicals and materials are concerned. This information, however, will become increasingly available throughout the innovation stages. As a result, assessment tools, information and criteria need to evolve over time.

It is important to note also an economical evaluation is being made, demonstrating the business case of the innovation at the different stages. These aspects fall outside the scope of this document. Having said this, an assessment framework supported by data and tools allowing to identify the non-viable options as quickly as possible within any innovation process would be highly appreciated (fail fast, fail cheap).

To reach the goal of enhanced safety and increased product sustainability, the SSbD approach requires consideration of safety and sustainability aspects throughout the stage gate process introduced earlier in this report, starting from the ideation stage (taking into account a specific pre-defined use case) onwards as well as taking into account the full life cycle. To achieve this, a workflow of five activities is suggested (Figure 6) to successfully implement a Safe-and-Sustainable-by-design framework. In the following paragraphs 2.3.1 to 2.3.5 of this report we seek to show how these 'activities' of the SSbD process map seamlessly onto the existing stage gate process used widely in industry.

OVERVIEW OF FOCUS DIMENSIONS

I	Human health hazard
II	Environmental hazard and fate
III	Issues arising from recycling conditions based on specific substances
IV	Climate change
V	Resources and waste
VI	Biodiversity and ecosystems impacts
VII	Emissions into air, water, soil
VIII	Life cycle cost

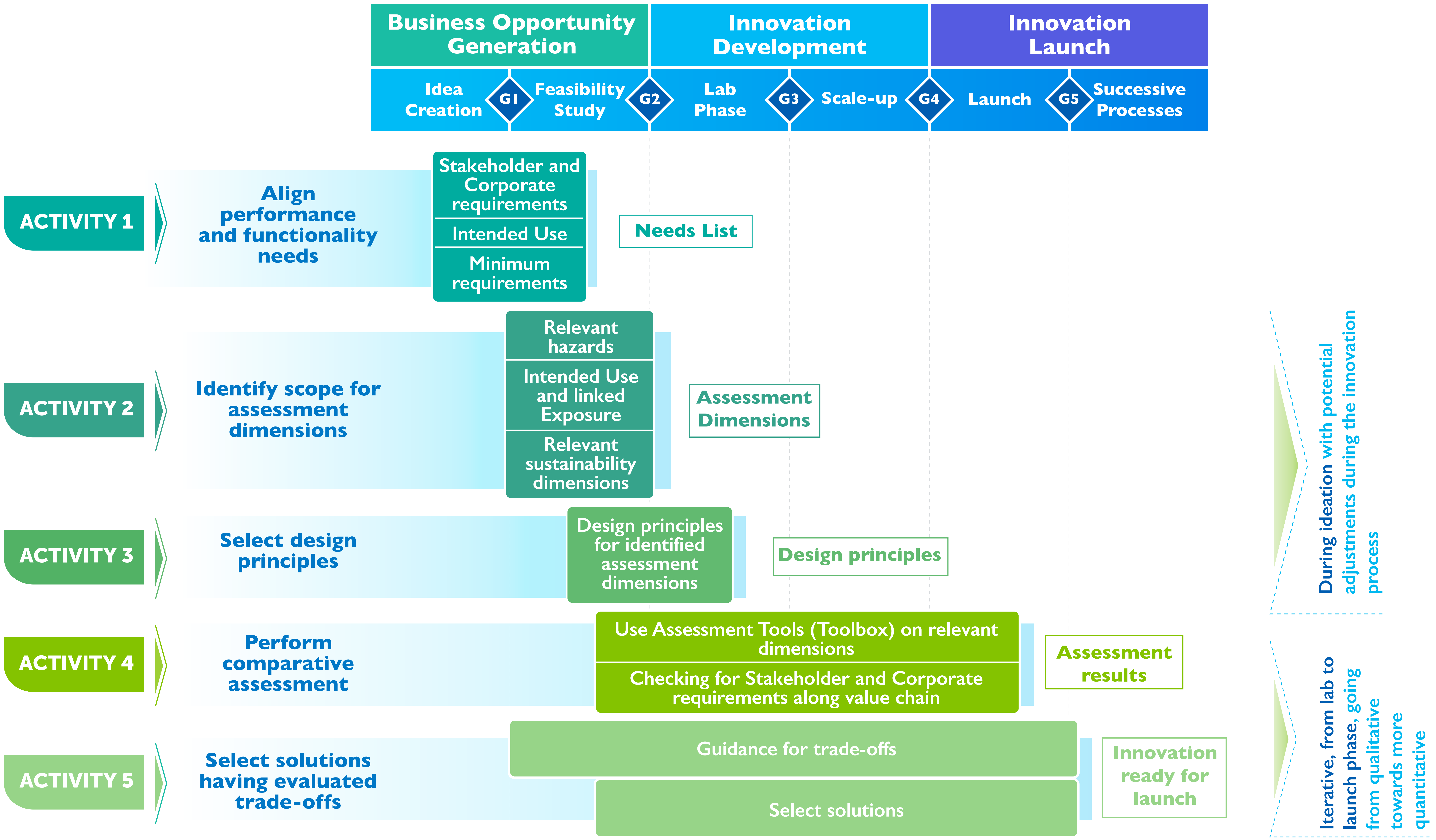


Figure 6. Suggested workflow (activities) for Safe and Sustainable-by-Design within an innovation process.

2.3.1 Idea Creation - going from Gate 1 to Gate 2

Idea creation, idea generation or even 'ideation' as it may be referred to is the entry point to the process. Ideas can come from a variety of sources and the active creation of new ideas is often deployed to support company strategy and to meet specific customer or market needs. Increasingly, companies are deploying tools such as the aforementioned PSA methodology by the WBCSD[20] and its updates to assess the overall sustainability of their product portfolio as a key driver for the selection of areas for innovation projects. Ideas can fall in different categories such as 'incremental' developments or more 'breakthrough' developments but the general concept of a stage gate innovation process can be applied in the majority of cases. Of course, much more may already be known about chemicals and materials that fall into the category of 'incremental' developments than for the ones that would qualify as 'breakthrough' developments, hence comparative data on structurally similar chemicals may be more readily available for incremental improvement projects.

During the idea phase, the key points to be addressed in the SSbD framework are associated with Activity 1 – aligning the performance and functionality needs:

- listing stakeholder and corporate requirements
- identifying the intended use
- determining the minimum requirements

These tasks correlate very closely with the beginning of the stage gate process where the idea is created and an initial understanding of why this project should be progressed is formed. At this early stage it is required to know what the problem to be addressed is, what use the new development is intended for and what is already known about the minimum requirements. The output from this activity will be a list of the identified needs which must be met for a viable project.

2.3.2 Feasibility Study - going from Gate 2 to Gate 3

Once an initial idea has been identified and a first screening has been conducted, companies will generally commit resources to perform both market and technical feasibility ananlyses, and screenings for issues of safety or sustainability. Gathering insights from different perspectives, this is the appropriate stage to consider whether the project 'makes sense' to pursue. Some companies will conduct preliminary market assessments and scoping experimentation to check the project's likelihood of success. Since there is some resource deployed at this stage, it is appropriate to also execute the second activity of the SSbD process in conjunction: Activity 2 - identify the scope of the assessment dimensions:

- identify relevant hazards
- based on the intended use, identify the linked exposure
- list the relevant sustainability dimensions

Predicitve models should be applied, especially in the context of incremental improvement projects (support of AI, data modelling etc.) Towards the end of the feasibility stage, there should be an accurate understanding of what the development targets are, both from a technical and market perspective but also from a Safe and Sustainable-by-Design perspective. The target setting for the Safe and Sustainable-by-Design objectives is correlated by the design principles. In any event, before entering the laboratory or development phase of a project, a clear understanding of all design principles is required. From an SSbD perspective this means the completion of Activity 3 – select the design principles.

2.3.3 Laboratory or Development Phase - going from Gate 3 to Gate 4

In the stage gate process the decision to start laboratory development is the major Go/No-Go decision point, as the phase will typically require deployment of significant resources. During this phase, options will be identified, experiments will be conducted, and scientific results will be generated. Candidate solutions will be developed. This is where the use of assessment tools will become important as solutions developed will be considered against their potential to meet technical requirements, market needs and against the relevant SSbD assessment dimensions.

At this stage, Activity 4 should be carried out - Perform comparative assessment:

- use assessment tools on relevant dimensions, typically NAMs that can compare conventional and new solutions, but not necessarily using regulatory Test Guidelines that could give definitive classification by CLP criteria, and not assessing all REACH data requirements.
- checking for stakeholder and corporate requirements along the value chain

As different candidate solutions are assessed, a more accurate evaluation of the potential trade-offs which may occur for each candidate solution and versus any incumbent solution which may be targeted for substitution by the new development becomes necessary. Here, Activity 5 is well suited to support decision taking - select solutions having evaluated trade-offs:

- guidance for trade-offs
- select solutions

2.3.4 Scale-Up & process development - going from Gate 4 to Gate 5

Frequently, laboratory scale developments will need to be 'scaled-up' to industrial production scale. Ideally, the general chemical route should not change if SSbD principles have been implemented already at the laboratory scale. Nevertheless, alternative chemistries and materials will handle this in different ways. In general, continued evaluation of the developed solutions will require to continue to be tested against the requirements and the continued use of the assessment tools will likely be required on any parameters which could change on scale-up.

In addition, the eco-efficiency analysis will emphasize which leverage has to be optimized during the process development (e.g. water consumption, solvent choice, biobased materials,…)

As the optimization efforts continue throughout this stage, Activities 4 and 5 are well suited to support respective decision taking when scaling up in preparation of the innovation's launch.

2.3.5 Launch

At launch, normally one final selected solution has been identified and should represent the best alternative amongst the evaluated options.

2.4 Safe and Sustainable-by-Design in action

The following chapter is going to describe the 5 activities defined along the innovation process in greater detail and provide examples on how the respective steps can be conducted. Where suitable, examples of methods and tools are provided as well. Given the differences in type and maturity of innovations, the examples provided can only showcase the different assessment steps. The topics material to a particular innovation, need to be identified individually and will determine the assessment scope and concrete screenings and tests to be conducted. An interdisciplinary action is required to scope and assess an individual innovation in the best possible and most efficient way. Early involvement and alignment of those disciplines is hence recommended.

2.4.1 Define performance and functionality needs – Activity 1

As described earlier, the starting point of many innovations is the identification of needs for improvement. These needs should address the most relevant or material safety and sustainability dimension. They can be found in the raw materials used, the production process applied or in the functionality and performance of a solution in its application or end-of-life, in other words considering the **intended use**. Adequately assessing the innovation needs therefore calls for the involvement of several disciplines covering all **stakeholder requirements** along the value chain for a particular intended use. Equally important are the **corporate requirements**, either resulting from the companies' sustainability strategy and /or business strategy aligned to their market segments. It is considered good practice to already flag which of those requirements can be considered as **minimum requirements**.

To ensure single improvement measures do not result in significant negatives in other areas, it is necessary to investigate all material dimensions along the life cycle of a given product-application-combination. In doing so, we suggest creating a list with all primary performance and functionality needs, which are directly linked to the solution in its application as well as all secondary needs resulting from stakeholders in the value chain, the legal framework and beyond, e.g., requirements from relevant eco-labels.

When looking into the performance and functionality needs, special care should be taken to identify those assisting as well as contradicting the desired transition of the EU Green Deal. Especially those contradicting the EU Green Deal targets should be a key focus for improvement of a solution.

Once the performance and functionality needs have been identified, the relevant dimensions for the SSbD assessment can be selected, according to activity 2.

2.4.2 Assessment Dimensions – Activity 2

For SSbD the key assessment areas for new chemicals, materials, products, processes and services in their respective use are "safe" and "sustainable".

2.4.2.1 Key dimensions to assess safety starting from relevant hazards

Under the key word "safe" we suggest considering the dimensions listed below, looking into **hazard** properties covering substances of very high concern as well as other categories amongst those that the CSS identified "the most harmful chemicals"[9], and other hazardous substances with a focus on consumer products.

As elaborated in 2.4.4, during ideation and feasibility phases, the design principles steer the innovation away from hazardous substances. The assessment of the following list by in-silico NAMs (based on structural similarity) should include a careful evaluation of the improvement potentials throughout the development phase, and may involve more targeted comparative testing by in-chemico and in-vitro NAMs during the lab phase:

Human health hazards (focus dimension 1):

- Global Harmonised System (GHS) carcinogenicity cat. 1A/1B/2 (H340/H341)
- GHS germ cell mutagenicity cat. 1A/1B/2 (H350/H351)
- GHS reprotoxicity cat. 1A/1B/2 (H360/H361/H362)
- Endocrine disruption cat. 1/2 according to the Classification, Labelling and Packaging (CLP) Regulation (H380/H381)
- GHS respiratory sensitizer cat.1 (H334)
- GHS Target organ systemic toxicity – single exposure cat. 1/2/3 (H370/H371)
- GHS Target organ systemic toxicity – repeated exposure cat. 1/2 (H372/H373)
- GHS skin sensitizer cat. 1A/1B (H317)
- GHS acute toxicity (dermal, oral, inhalation) cat. 1/2 (H310/H300/H330)
- GHS acute toxicity (dermal, oral, inhalation) cat. 3/4 (H311/H312/H301/H302/H331/H332)
- GHS aspiration toxicity cat. 1 (H304)
- GHS skin corrosive substances (H314)
- GHS skin irritation substances (H315)
- GHS serious eye damage / eye irritation (H381/H319)

Environmental hazards (focus dimension 2):

- Substances determined as very persistent and very bio-accumulative (vPvB) or persistent, bio-accumulative, and toxic (PBT) in the environment according to the CLP Regulation (H440/H441)
- Substances determined as very persistent and very mobile (vPvM) or persistent, mobile, and toxic (PMT) in the environment according to the CLP Regulation (H450/H451)
- Endocrine disruptors Cat. 1/2 according to the CLP Regulation (H430/H431)
- GHS ozone depleting substances (H420)
- GHS chronic aquatic toxicity cat. 1/2/3/4 (H410/H411/H412/H413)
- GHS acute aquatic toxicity cat. 1 (H400)

Physical hazards:

- Explosives
- Flammable gases, liquids and solids
- Oxidizing gases, liquids, solids
- Gases under pressure
- Self-reactive substances
- Pyrophoric liquids, solids
- Self-heating substances
- Substances which in contact with water emit flammable gases
- Organic peroxides
- Substances corrosive to metal
- Desensitized explosives

2.4.2.2 Intended Use and linked Exposure

In any case of innovation, the identification of the intended use of the new chemical, material, process or service to be developed (also already clarified in activity 1) is essential when determining the scope of the assessment dimensions in activity 2. The intended use comes with certain exposure scenarios that will have an influence on the form of the design principles to be applied. We differentiate here between "industrial process use" on the one hand and "consumer use incl. professional use" on the other. **"Industrial process use"** is the use of the product/application combination of the chemical/material in question in an industrial process (chemical plant, engineering plant etc.) using state of the art measures regarding risk management and labor safety (e.g. ideally processes in full containment). In "consumer use incl. professional use" the chemical/material in question is used in a specific product-application combination in the following scenarios: either by a) the end consumer in day-to-day life without any specific protective measures (i.e. without personal protective equipment) and/or knowledge on the chemical/material present in the solution or by b) professionals trained in the use of the chemical/material in question with a basic level of specific protective measures taken (i.e. use of personal protective equipment) and/or with knowledge on the chemical/material present in the solution.

2.4.2.3 Key dimensions to assess sustainability

Under the key word "sustainable", we are suggesting the following dimensions from all three pillars of sustainability to be considered (non-exhaustive list). Hereby, we differentiate between focus dimensions, minimum requirements, and additional dimensions, as defined above.

The dimensions become relevant for the assessment if raw materials, production prcesses, the use case or end-of-life show material impact. The assessment should include a careful evaluation of the improvement potentials during ideation and throughout the development phase:

Environment:

- Issues arising from recycling based on specific substances and recycling technology applied (focus dimension 3)
- Climate change (focus dimension 4)
- Resources and waste (focus dimension 5)
- Biodiversity and ecosystem impacts (focus dimension 6)
- Emissions into air, water, soil (focus dimension 7)
- Protection of water and marine resources

Society:

- Workers
  - › Health and safety (minimum requirement)
  - › Human rights, child labor, and forced labor (mimimum requirement)
  - › Working conditions (e.g., remuneration, gender equality, fair salary, working hours)
  - › Freedom of association and collective bargaining
  - › Equal opportunities and discrimination
- Local communities
  - › Access to basic needs for human right and dignity (e.g., health care, clean water and sanitation, health food, shelter)
  - › Health and safety of local community's living condition (minimum requirement)
  - › Public Health
  - › Local employment and job creation
  - › Community engagement
- Consumers
  - › Impact on consumer health and safety (minimum requirement)
  - › Affordability and competitiveness
- Value chain actions not including consumers
  - › Fair competition
  - › Promoting social responsibility
  - › Supplier relationships
  - › Respect intellectual property rights

Economy:

- Profitability
- Life cycle cost (including cost for production) (focus dimension 8)
- Resilience
- Economic and technical sovereignty

2.4.2.4 Other key dimensions

Finally, in accordance with the PSA 2.0 methodology, we suggest two additional dimensions to be considered for assessment:

- Corporate requirements (minimum requirement)

- Stakeholder expectations (minimum requirement)

Both type of requirements, however, are often influencing the performance and functionality needs, and it is recommended to already consider them in Activity 1.

2.4.3 Design Principles – Activity 3

The overarching principle in innovating towards a pre-determined performance or functionality for a defined use case is to « *significantly improve in at least one of the dimensions, considered under i.e., safety or sustainability, without significant negative effects on any of the other dimensions, compared to incumbent solutions* » always in full respect of certain minimum requirements, e.g., regulation and international conventions. This will lead to an iterative improvement process progressively pushing the performances on "safe" and "sustainable" over time. Of course, innovation will not only be about improvement steps, but is also happening from scratch and looking for disruptive ideas.

For the three focus dimensions, considering aspects of safety and following **design principles** that focus on hazards and exposure are recommended to be considered in the innovation phase. Considering these in the early stages will help the aforementioned fail-fast approach and inform and shape the successive trade-off decisions.

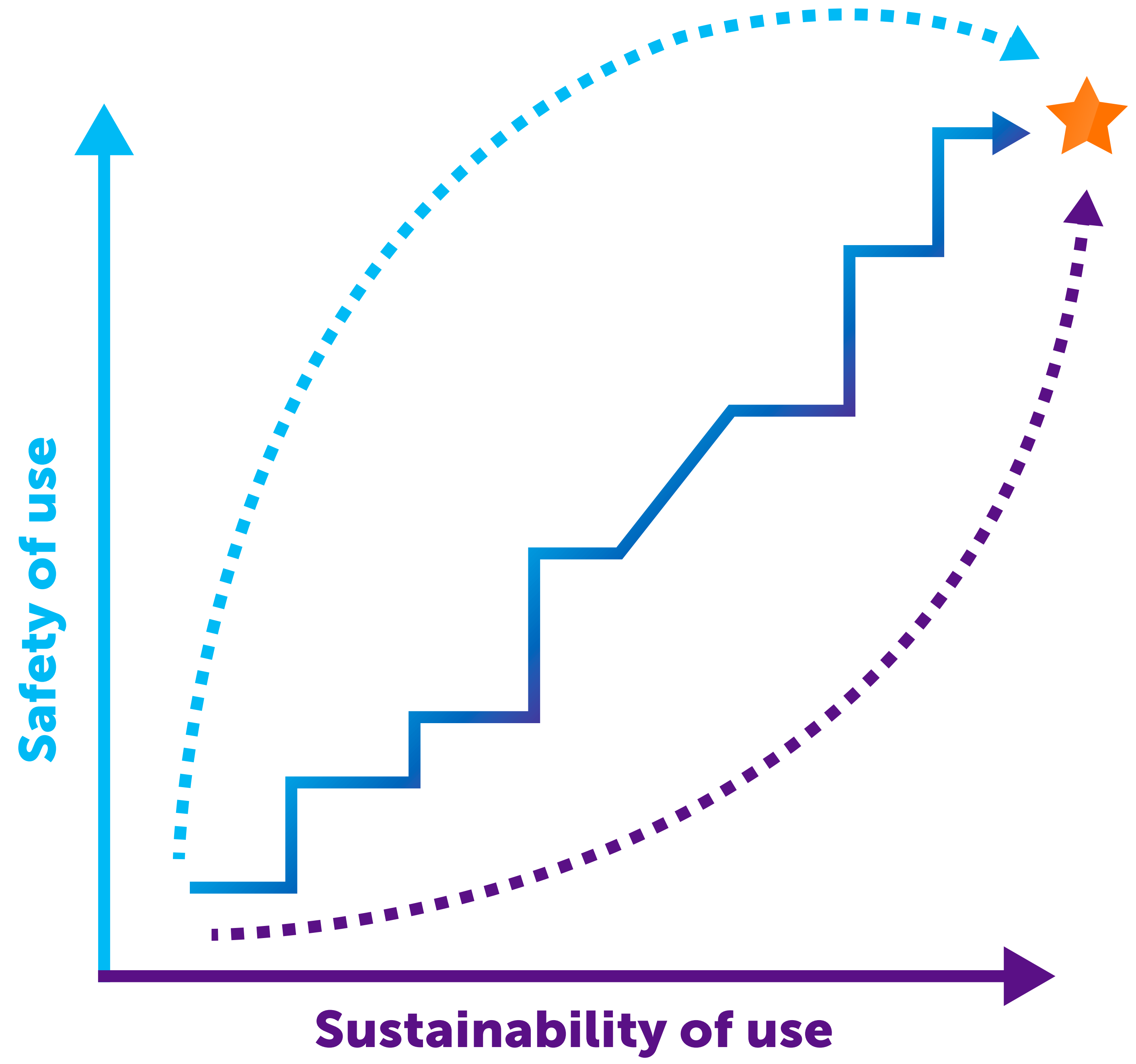


Figure 7. Schematic depiction of iterative steps of improvement (violet) or from scratch improvement (blue) in the dimensions "safety of use" and "sustainability of use".

ACTIVITY 3

Select design principles (list of recommendations)

	Dimension	Sub-dimension	Substance Category	Design principle
Safety	Human Health hazard (Focus dimension I)	Carcinogenicity	Cat. 1A and 1B	I
			Cat. 2	II
		Germ cell mutagenicity	Cat. 1A and 1B	I
			Cat. 2	II
		Reproductive/developmental toxicity	Cat. 1A and 1B	I
			Cat. 2	II
		Endocrine disruption (human health)	Cat. 1	I
			Cat. 2	II
		Respiratory sensitization	Cat. 1	I
		Specific target organ toxicity - repeated exposure (STOT-RE)	Cat. 1	I
			Cat. 2	II
		Specific target organ toxicity - single exposure (STOT-SE)	Cat. 1 and 2	II
			Cat. 3	III
		Skin sensitization	Cat. 1A and 1B	II
		Acute toxicity (dermal, oral, and inhalation); Aspiration hazard cat.1; Skin corrosion; Skin irritation; Serious eye damage/ eye irritation		III
	Environmental hazard and fate (Focus dimension II)	Very persistent and very bio-accumulative (vPvB), persistent, bio-accumulative; and toxic (PBT);		
		Very persistent and very mobile (vPvM); persistent, mobile, and toxic (PMT)		I
		Endocrine disruptors	Cat. 1	I
			Cat. 2	II
		Ozone depleting substances		II
		Chronic aquatic toxicity	Cat. 1 and 2	II
			Cat. 3 and 4	III
		Acute aquatic toxicity	Cat. 1	III
	Physical hazard	Explosives; Flammable gases, liquids and solids; Oxidizing gases, liquids, solids; Gases under pressure; Self-reactive; Pyrophoric liquids, solids; Self-heating; In contact with water emits flammable gas; Organic peroxides; Corrosivity; Desensitized explosives		III

Figure 8. Assessment dimensions on safety, with the related design principles on a substance category level.

Design principle I: Risk assessment and management CMR cat. 1, respiratory sensitisers cat. 1, STOT-RE cat. 1, vPvB, PBT, vPvM, PMT and ED cat. 1 substances

- For the anticipated production process(es):
  - Eliminate or minimise adverse effect through reduction or substitution of hazards and/or exposure
  - Analyse and avoid as much as possible the use of substances with the relevant hazards
  - Consider value chain specific regulations.
- For the anticipated use phase and end-of-life:
  - For intended consumer use, do not develop solutions with characteristics qualifying or likely to be classified as the relevant hazards
  - Follow value chain specific regulations

Design principle II: Risk assessment and management CMR cat. 2, ED cat. 2, STOT-RE cat. 2, STOT-SE cat. 1&2, skin sensitisation cat. 1, ozone depleting substances, chronic aquatic toxicity cat. 1&2 substances

- For the anticipated production process(es):
  - Reduce adverse effect through reduction of hazards and/or exposure
  - Analyze and try to avoid the use of substances with the relevant hazard classifications

  - Consider value chain specific regulations
- For the anticipated use phase and end-of-life:
  - Avoid the development of consumer solutions with characteristics qualifying or likely to qualify for a classification as the relevant hazards
  - Follow value chain-specific regulations

Design principle III: Risk assessment and management STOT SE cat. 3, Acute toxicity, aspiration hazard cat. 1, skin corrosion, skin irritation, serious eye damage, eye irritation, chronic aquatic toxicity cat. 3&4, acute aquatic toxicity cat. 1 substances and substances having a physical hazard

- For the anticipated production process(es):
  - Consider risk reduction through limitation of hazards and/or exposure
  - Analyze and try to avoid the use of substances with the relevant hazards
  - Consider value chain specific regulations
- For the anticipated use phase and end-of-life:
  - Monitor the development of consumer solutions with characteristics qualifying or likely to qualify for a classification as the relevant hazards
  - Follow value chain-specific regulations

ACTIVITY 3

Select design principles (list of recommendations)

		Dimension	Sub-dimension	Design principle
Sustainability	Environment	Issues arising from recycling conditions based on specific substances (Focus dimension III)		IV
		Climate change (Focus dimension IV)	Climate change adaptation Climate change mitigation Energy	V
		Resources and waste (Focus dimension V)	Resources inflows, including resource use Resource outflows related to products and services Waste	VI
		Biodiversity and ecosystems impacts (Focus dimension VI)	Direct impact drivers of biodiversity loss Impacts on the state of species Impact on the extent and conditions of ecosystems Impacts and dependencies on ecosystem services	VII
		Emissions into air, water, soil (Focus dimension VII)	Emission into air, water, and soil Pollution of living organisms and food resources Substances of concern / Substances of very high concern	VIII
		Protection of water and marine resources	Water withdrawals, consumption, and use Water discharges in water bodies and in the oceans Extraction and use of marine resources	

Figure 9. Assessment dimensions on environmental sustainability, linking to the respective design principles for innovation.

For the 5 focus dimensions which are covering the aspects of environmental sustainability the following **design principles** are to be considered.

Design principle IV: Issues arising from recycling based on specific substances and recycling technology applied.

- Think of the planned EPR[23] schemes and recycling routes which can identify the substances hampering the recycling
- For the anticipated production process(es):
  - Analyse and try to avoid the use of substances considered to hamper collection, sorting, and recycling
  - Consider value chain-specific regulations
- For the anticipated use phase and end-of-life:
  - Avoid utilisation or development of solutions hampering recycling
  - Follow value chain specific regulations
  - Consider waste related aspects in order to avoid obstacles in waste transports and end of waste status

Design principle V: Climate change

- Select raw materials and processes that minimise the generation of greenhouse gases
- Select and/or develop (production) processes with minimised generation of greenhouse gases, e.g. the possibility of green heat networks, electrification
- Develop products which enable greenhouse gas emission savings down stream (use phase and end-of-life)

Design principle VI: Resource use and waste

- Select materials and processes that minimise the generation of waste
- Select materials and processes that use/allow the use of sustainably[24] sourced biobased feedstock and/or sustainably sourced circular feedstock
- Select materials that have (where appropriate) an increased durability or enable product sharing, reduced maintenance or a commercial 'afterlife'
- Compose products in a way which - as much as meaningful– strive for recyclability
- Compose products in a way which - as much as meaningful – strive for biodegradability
- Match the raw material selection to the capabilities of the waste management operations in the intended market
- Select materials and processes that reduces the abiotic depletion potential[25]

Design principle VII: Biodiversity and ecosystems impacts

- Select raw materials that minimise the negative impact on biodiversity and the overall ecosystem (e.g. minimise deforestation/ mono cultures/… when using renewable raw materials)
- Innovate raw materials (and possibly their integration into value chains) with a more benign production process, and/or with a regenerative impact on biodiversity and ecosystems
- Select and/or develop (production) processes that minimise the negative impact on biodiversity and the overall ecosystem (e.g. asset-associated land use, emission control e.g. cooling water outlet, general waste generation…)
- Aim for the development of products that have a positive effect on biodiversity and ecosystems (e.g. products that help regenerate biodiversity such as when the renewably sourced raw materials can come from multicultures instead of monocultures; products that are biodegradable to keep carbon in loop (digest by bacteria), e.g. check what can be transferred to white biotech technology instead of e.g. land-use based raw material generation

Design principle VIII: Emission into air, water, soil

- Select raw materials and processes that minimise the generation of emissions (e.g. VOCs, TOCs, acidification, overfertilization, heavy metals…)
- Select and/or develop (production) processes with minimised generation of emissions (e.g. VOCs, TOCs, acidifcation, overfertilization, heavy metals …)
- Develop products which enable emission savings down stream (use phase and end-of-life)

For the focus dimensions, which are covering the aspects of societal and economic sustainability the following **design principles** should be considered in the ideation phase.

Design principle IX: Life cycle cost

- Select raw materials and processes that allow for cost savings over the life cycle of a product, process or service through:
- Savings on e.g. use of energy, water and fuel
- Savings on e.g. maintenance and replacement
- Savings on e.g. recycling or disposal costs

2.4.4 Comparative assessment – Activity 4

The innovation phases of experimental development and scale-up (mainly between Gates 3 and 5) including testing and validation of the different innovation candidates is an iterative process comparing the different alternatives, often qualitatively, against the requirements defined at the beginning, as well as the incumbent solution on the market. Focussing on the previously defined requirements, an informed decision taking should enabled supporting a "fail-early-fail-cheap" logic.

In doing so, the number of candidates typically is going down with increasing technical readiness level (TRL), leaving only a small number of promising candidates going into the scale-up phase.

In line with the prioritized requirements in the previous steps, an individual assessment strategy should be developed, addressing must-have requirements from the early innovation stages onwards. The strategy developed should reflect the best available methods for selecting the best alternative regarding the relevant requirements. Nonetheless, for some requirements there are no methods available

ACTIVITY 3

Select design principles (list of recommendations)

		Dimension	Sub-dimension	Design principle
Sustainability	Societal	Workers	Health and safety (minimum requirement)	
			Human rights / child labor / forced labor (minimum requirement)	
			Working conditions (remuneration, gender equality, fair salary, working hours …)	
			Freedom of association and collective bargaining	
			Equal opportunities / discrimination	
		Local communities	Access to basic needs for human right and dignity (healthcare, clean water & sanitation, healthy food, shelter)	
			Health and safety of local community's living condition (minimum requirement)	
			Public Health	
			Local employment / Job creation	
			Community engagement	
		Consumers	Impact on consumer health and safety (minimum requirement)	
			Affordability & Competitiveness	
		Value chain actions not including consumers	Fair competition	
			Promoting social responsibility	
			Supplier relationships	
			Respect intellectual property rights	
	Economical	Profitability		
		Life cycle cost (Focus dimension VIII)		IX
		Resilience		
		Economic and technical sovereignty		

Figure 10. Assessment dimensions on societal and economic sustainability, linking to the respective design principles for innovation

for all TRLs or it is sufficient to apply only a few out of many available methods to select the better alternative.

Good-to-have requirements may be added to the assessment strategy as well with a lower priority or at a later point in time. Any assessment strategy needs to consider the relevant elements of safety (e.g., human- and environmental- toxicological endpoints which are material to the targeted application), sustainability (e.g., material aspects for the innovation's footprint and related sustainability benefit along the full life cycle), and performance (e.g., specific properties, needed for the proper functioning within the targeted application) as must have requirements.

Out of the eight dimensions identified as focus dimensions (Toxicological potential for humans, Toxicological potential for the environment, Risks resulting from recycling, Climate change mitigation, Resource use of renewable and circular feedstock, Reduction of emissions into air, water, soil, life cycle cost), which should always be assessed looking for a significant improvement, five cover the product's sustainability. Two other focus dimensions are attributed to aspects of safety (chapter 2.4.2). Comparative assessments should be done for the same functional and/or performance basis for the innovation relative to the incumbent solution.

As the innovation evolves from early feasibility studies, through detailed development in the laboratory, to scale-up the screening and/or test methodologies applied may evolve also. Typically, they evolve from lower levels of specificity and accuracy in predicting results to increased levels. Recognizing this interplay between applicable screening / test methodologies and the technical readiness level (TRL) is an important lever to optimize the informative value already at early innovation stages and fostering a targeted fail-early-fail-cheap mechanism.

A hands-on guidance on what and how to assess innovations will be provided in this chapter.

2.4.4.1 Preparing for a practical assessment - must-have requirements and good-to-have characteristics

For an innovation product to be successful on the market, several requirements need to be fulfilled, which depend highly on the final application and market in focus. When designing a product, those requirements define to a large extent the characteristics and specification of the final product, which need to be respected during the innovation process and the development of the product. In many cases there will be requirements which must be fulfilled – must-have requirements – and characteristics which would be beneficial to be fulfilled – good-to-have characteristics. Through such prioritization, focus areas for the assessment can be derived:

Exemplary must-have requirements can result from:

- Legally binding standards on safety, sustainability or performance

During activity 4, it is recommended good practice to continue **checking for stakeholder and corporate requirements along the value chain**. These requirements may be sorted again in must-have requirements or good-to-have characteristics:

- Up-coming regulatory changes on safety, sustainability or performance
- Customer- or sector-specific expectations e.g., on performance such as
  - › Biodegradability
  - › Lower hazard classification
  - › Physicochemical properties
- Individual corporate requirements e.g., all new products should be more sustainable than incumbent solution

2.4.4.2 Tools/indicators to enable informed decision taking

a Requirements for tools

- Clear definition of functional units in scope
- Applying a holistic view through life-cycle thinking
- Applying similar quality of input data ensuring similar quality of assessment outcome (transparency on data quality and/or assumptions made)
- Suitability for the specific molecule / material system of interest ➞ reliability of predictability or assessment
- Comparability of results for different innovation candidates (apply similar system boundaries and similar methods) ➞ enables narrowing down on the better alternative
- Reliability in terms of no false positives or negatives
- Predictability on higher tier testing and more complex assessments
  - › if possible with non animal methods
  - › if possible with low data availability for sustainability assessment

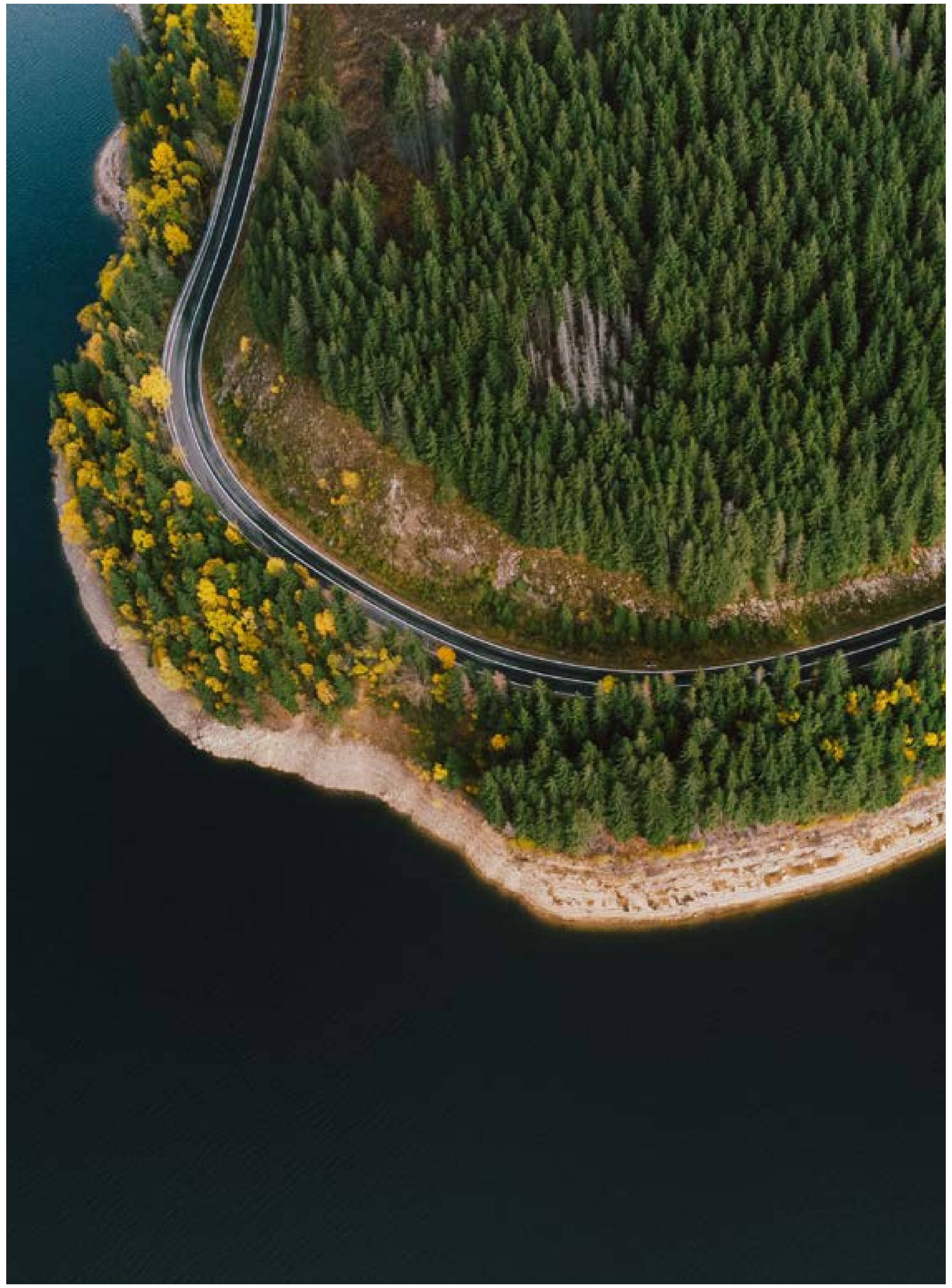
- Scenario calculations
- Optional aggregation to single score results
- Alignment with ISO standards
- Cost efficiency

b Groups of tools / examples of tools:

- Hazard assessment

The development of new chemicals or materials requires a thorough assessment of hazards associated with the respective solutions in their intended application. However, many of the required hazard input data for a full-blown SSbD assessment are not yet available at an early innovation stage, especially for new chemicals and materials since the uncertain commercial value of the project does not support untargeted screening for all potential hazards. Instead, a hot-spot analysis can trigger comparative hazard assessment with screening methods of limited predictivity. For the screening of hazards several types of tools have been developed and are still being developed further.

Generally, tools for (early) screening and regulatory testing can be differentiated. They differ in the level of validation, but already early screenings can be very helpful indicators to further down select one alternative over another. Many of these methods belong to the group of rapidly evolving New Approach Methods (NAMs) and include, for example, in silico approaches (prediction with (quantitative) structure-activity relationship (Q)SAR or read-across), in vitro methods, integrated approaches to testing and assessment (IATA), adverse outcome pathways (AOPs), a combination thereof and others. Furthermore, in vivo methods can be applied, where useful. Nonetheless, the number of methods available and the predictability of the available methods differs significantly from hazard endpoint to hazard endpoint, as illustrated in Figure 11. For example, in the case of germ cell mutagenicity a number of different test methods over all TRLs are available delivering full insights on the particular hazard. The evaluation of STOT RE or SE, in contrast, is rather complicated, as for many of the TRLs no conclusive, or only partially conclusive methods are available. Respective lacks need to be considered in developing the test strategy. When developing a specific assessment strategy for an individually developed chemical or material, a suitable set of assessment tools supporting a resilient evaluation and down-selection of candidates should be chosen.



Level of predictivity increases

Effort	DAYS			WEEKS				MIN. 12 MONTHS
	SCREENING (only used for early (eco)tox alert identification)				**REGULATORY TESTING** (up to EU REACH annex VIII requirements)			**AVAILABLE DATA**
Hazard Assessment tools / Examble Hazard End points	**New Approach Methodology (NAMs)**				**New Approach Methodology (NAMs)**			
	in silico testing/prediction on structural similarities (structure from design specs. or measured)	single *in vitro* test	combined *in vitro* tests	*in vivo*	*in vitro* (OECD GD plus GLP)	combined *in vitro* test (OECD GD plus GLP)	*in vivo* (OECD GD plus GLP)	flagging for undesired effects
Germ cell mutagenicity	Full	Full	Full	No	Full	No	Full	Full
STOT RE / SE	No	No	No	Partial	No	No	Full	Full

Figure 11. Example types of methods for hazard assessments within activity 4.

- Exposure assessment

To conduct a risk screening in early innovation stages, basic information on potential hazards associated with a chemical as well as its way of production, way of use and end-of-life are required, which in many cases are not yet available.

For early innovation stages, the down-selection process to the best alternative is still ongoing. As a result, the raw materials, their production process, as well as the innovation's own production process and potential additional down-stream processes are not fixed. Consequently, a lifecycle inventory cannot be established, and early innovation phases call for simplified approaches to assess a potential exposure, such as hot-spot analysis, as can be done with TNO's Hot-Spot Scan.

Once required data become available for higher TRLs, the risk of different alternatives in production, use and end-of-life can be compared to each other. It is important, though, to ensure comparable assumptions and equivalent data sets going into the calculation of the Risk Characterization Ratio (RCR) by "normalizing" the Risk Mitigation Measures (RMM), which are closely linked to the innovation's properties and exposure situations.

A possibility to "normalize" RMMS is the usage of Sector-specific knowledge on exposure, e.g., available from ECHA's use maps, which support an initial workers exposure assessment (SWEDs), consumers exposure assessment (SCEDs) and environmental exposure assessment (SPERCs).

- LCA: "Prospective" early evaluation / Environmental impact assessment

When assessing the environmental impacts of innovation candidates, life-cycle thinking should be applied, covering all stages of a product system including resource extraction, raw material production, manufacturing, use and end-of-life. This is important to avoid sub-optimal solutions that mitigate environmental impact in one part of the lifecycle but increases the impact in another part leading to an overall worse environmental impact.

Furthermore, holistic environmental thinking should be applied considering all relevant different environmental dimensions (chapter 2.4.2). The must-haves vs. the nice-to-haves (chapter 2.4.4.1) and the trade-off system (chapter 2.4.5) plays in to determine which of the environmental dimensions carry most weight for a certain innovation project, which ultimately will depend on the specific value chains. E.g., climate impact is likely to be a key environmental dimension that carries a lot of weight in many assessments, while land use and associated biodiversity aspects can be important for value chains involving renewable biobased resources. The geographical scope can also be important for environmental dimensions which have more local impacts, e.g., a water use assessment should ultimately consider specific local circumstances.

Life Cycle Assessment (LCA) is hence a holistic approach that can be used to assess many environmental impacts in parallel. The results can be transferred to recommendations, probably with additional application of normalization and weighting. At the early stages 2-3 of the innovation process, if there is limited information about the candidates, a qualitative screening type of LCA can be applied, e.g., involving checklists, proxy data and an interview type of approach by experienced sustainability specialists who are familiar with the typical hot spots of certain value chains. When chemistry and supply chains are known, a quantitative life cycle assessment can be made to improve robustness of the assessment.

Through a Life Cycle Impact Assessment (LCIA) an LCA can generate an eco-footprint covering several different environmental impact categories, including e.g., climate impact (carbon footprint) and resource use (see Figure 12). For each environmental impact category there can be different characterization methodologies available to do the LCIA, and these are normally available in commercial LCA software. ProScale and USETox are methods for integrating toxicity assessments of chemicals as impact in the LCIA assessment. ProScale considers additionally a risk mechanism behind the characterization of chemicals. The ProScale approach is a meaningful approach when the direct human toxicity within an LCA should be considered. ProScale E for Eco-toxicity assessments will be available soon and can be applied in the LCA context as well.

For communication purposes and to harmonize decision making, a weighting methodology can be applied to aggregate the different environmental impact categories into an overall environmental impact indicator (chapeter 2.4.5 – trade-offs).

There are ISO standards for LCAs, e.g., the ISO 14040 and ISO 14044 for LCAs, ISO 14067 for carbon footprints or ISO 14046 for water footprints available. Together for Sustainability (TfS) guideline for PCFs is a drop-in standard developed for the chemical industry and is based on the above-mentioned generic ISO standards. Interpretation and weighting are described in ISO 14074, and rules for communication of LCA results were published in the ISO 14020 series. The upcoming ISO 14076 Eco-Techno-Economic Analyses (eTEAs) can be helpful in the process evaluation.

Since the LCA depends on a higher number of datasets with high quality that are covering the different life cycle steps as manufacturing, use and waste treatment activities globally, a LCA needs also to deal with uncertainty, data quality, scenario assessments, etc. Moreover, the choice of LCA methodology, such as the way environmental impacts are allocated between by-products and waste that will be recycled, can have a significant impact on the results. It is therefore very important to carefully review the underlying LCA methodology and the data used to ensure fair comparison of different candidates and the correct interpretation of the results. Sector-specific guidelines such as the PCF guideline of Together for Sustainability (TfS) and even more specific rules derived from Product Category Rules (PCR) can be developed and applied. The iterative approach in combination with sensitivity analysis, scenario analysis and the evaluation of quality indicators can be used to address these uncertainties and support decision making in a meaningful way. The concept of significant improvements can also be applied to assess uncertainties and to support any claims.

Inputs for circularity indicators can also be generated with an LCA and complements the standard LCA environmental impact indicators by quantifying how much of the value chain is based on circular material and energy feedstocks, e.g. based on ISO/DIS 59020.

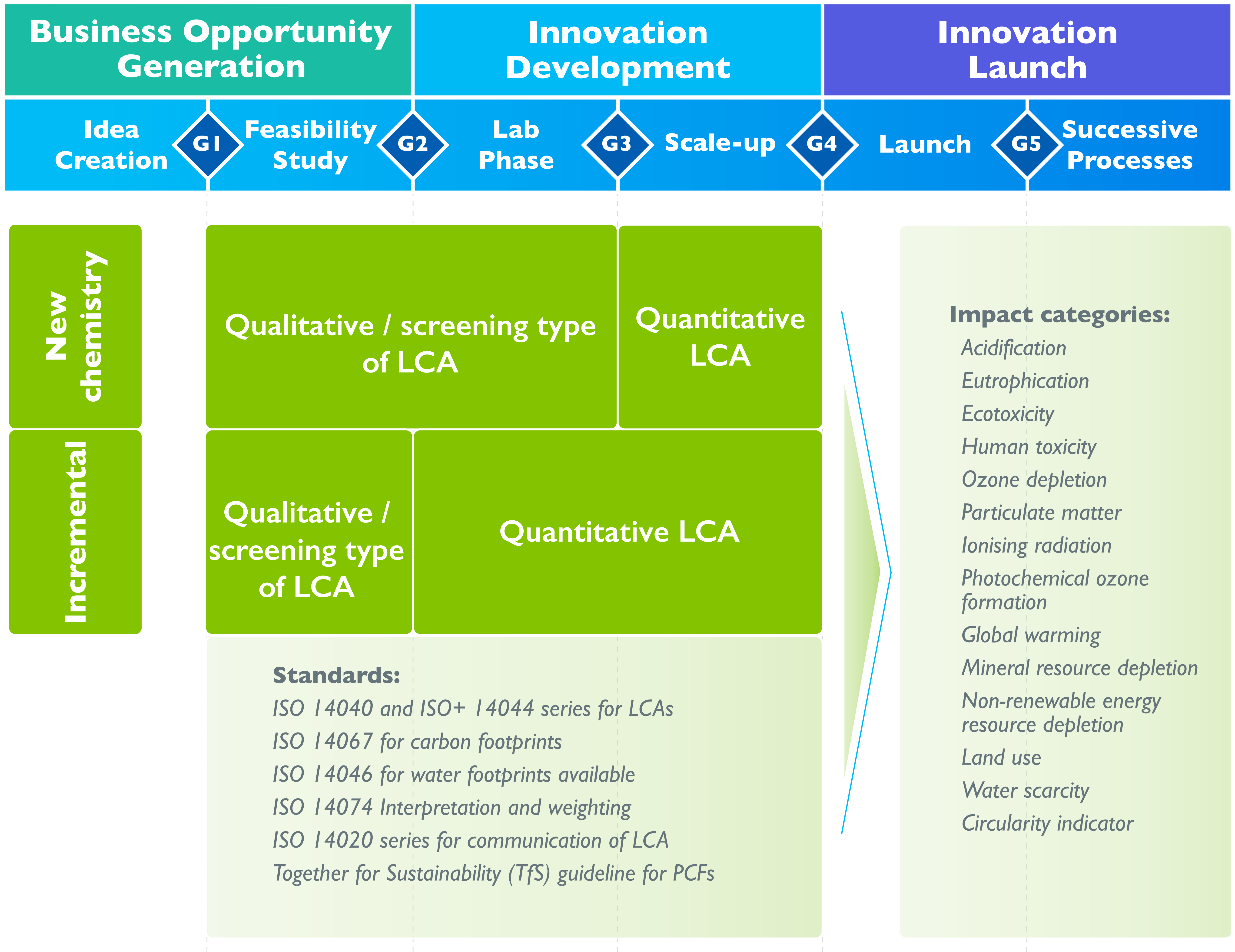


Figure 12. Example types of methods for life cycle assessments within activity 4.

It needs to be acknowledged that the toolbox for assessing the sustainability dimensions is at different levels of maturity and will need further development.

As indicated in Figure 12, depth and level of detail for the LCA strongly depends on the availability of data. This is drastically different for developments of new chemistries versus incremental improvements. Hence, it requires a case-by-case decision at which TRL an LCA assessment is feasible for a particular category. Similarly, the level of LCA quantification may differ significantly on an individual level.

- Socioeconomic impact assessment (to be developed in future)

ISO 14075 Social LCA can be the basis of further developments.

2.4.4.3 Example cases for illustration:

To illustrate the need for tailored assessment approaches, reflecting the type of innovation two vastly different examples are presented. The first example (Figure 13) depicts the testing strategy for the development of a new substance (break-through innovation), which typically involves limited data availability especially in the early phases of the innovation process as well as particularly high risk of failure for such attempts.

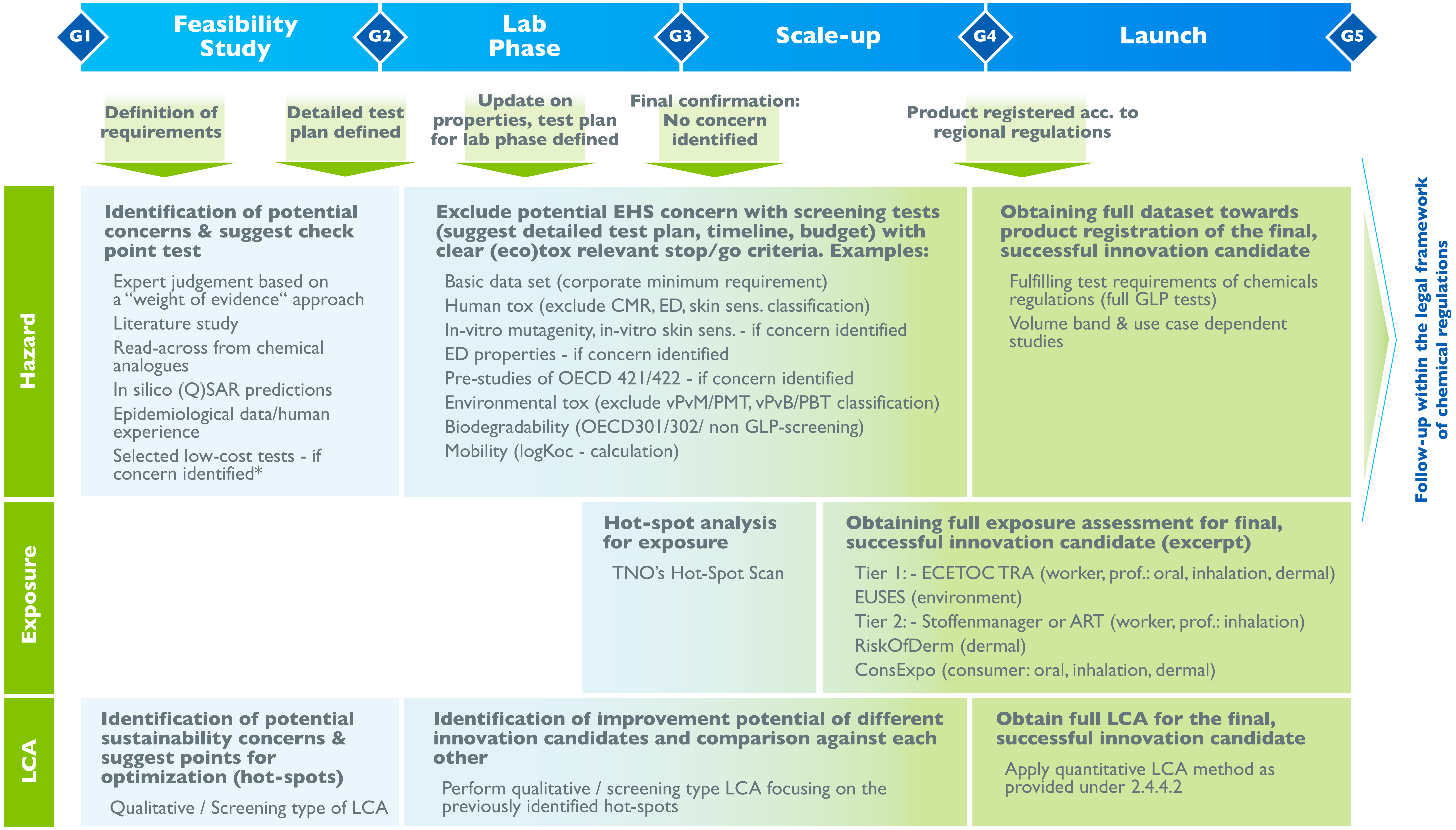


Figure 13. Exemplary assessment roadmap for new-to-the-world products and processes.

The second example (Figure 14) depicts the testing strategy for an incremental innovation, e.g., based on existing chemicals for a product re-design. In such cases, typically data availability through Safety Data Sheets (SDS) is given, for well-known components. In a re-design situation, also the use case and end-of-life situation are known quite well in many cases, which has a huge effect on the focus of the testing strategy.

The combination of dimensions ends up in a complete picture of the innovation process with respect to SSbD. It should be noted that some key dimension having a strong improvement can compensate for other dimensions of lower performance. In any case, the comparative assessment also includes an assessment to avoid significant negative impacts on other relevant dimensions.

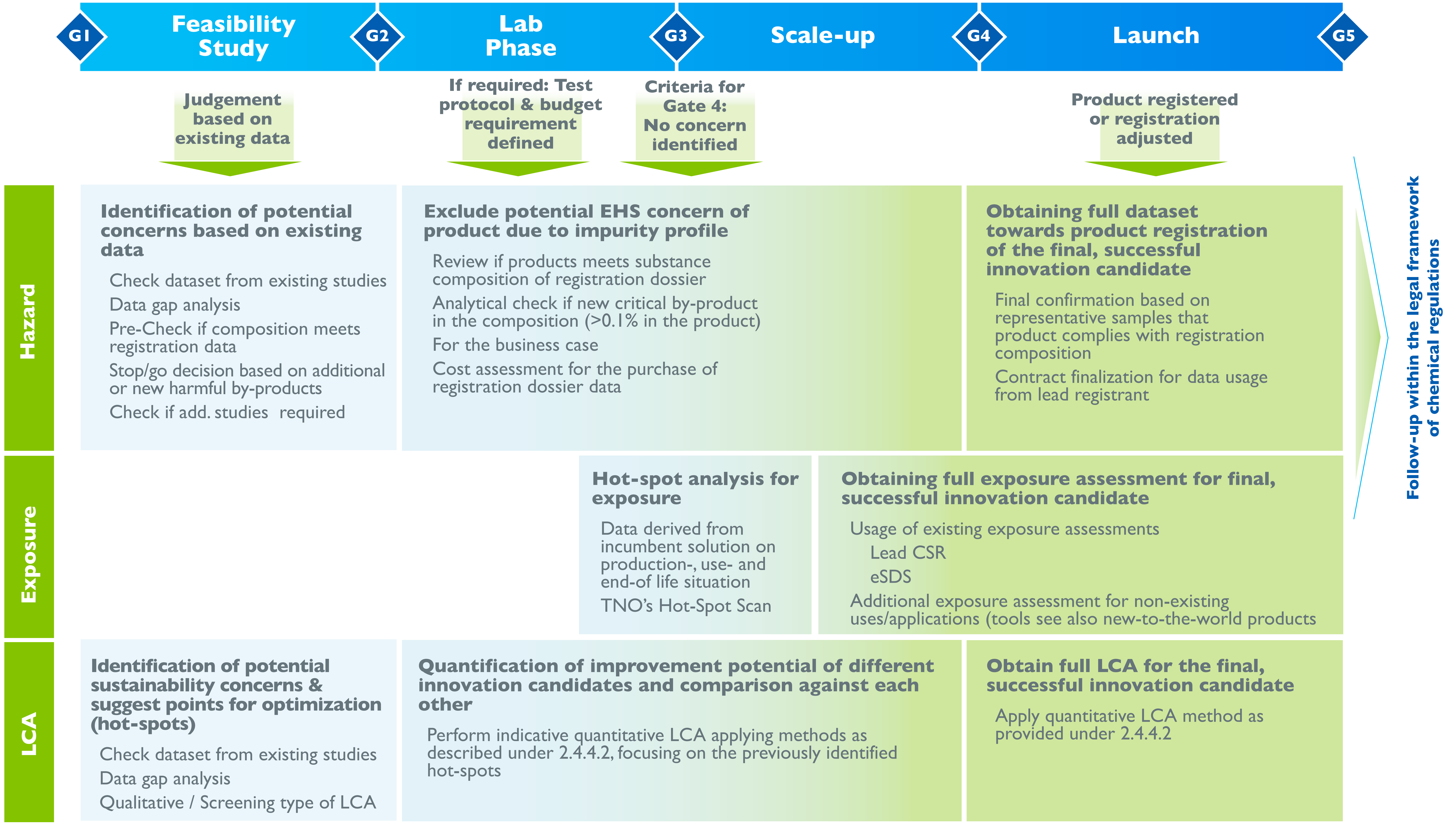


Figure 14. Exemplary assessment roadmap for (incremental) product (re-)design and processes.

2.4.5 Trade-offs – Activity 5

Selecting solutions or making choices on alternatives is an activity that runs through almost all stages of the innovation process. Seldomly a solution will present itself outstanding in all the relevant assessment dimensions for an intended product-application combination. Choosing between solutions and taking trade-off decisions are indeed more the rule, than the exception. That is why it is important that this guidance also spends some thought on the trade-off practices.

2.4.5.1 Introduction [WHY?]

What do well reputed sources tell us about the meaning of trade-offs? The Merriam-Webster dictionary refers to it as balancing of factors all of which are not attainable at the same time. The Cambridge dictionary defines trade-offs as an act to accept a disadvantage or bad feature in order to have something good and in the Brittanica we learn it is about a situation in which you must choose between or balance two things that are opposite or cannot be had at the same time.

Trade-off decisions are an essential building block on how progress is being made in society in general. The chemical industry is not an exception; most innovation involves trade-off decisions.

Any SSbD framework therefore needs to devote thought to innovation trade-offs, without becoming too prescriptive about the actual criteria.

The latter is considered to be part of the business strategies of the companies. Principles and red-line discussions are however welcomed, giving guidance to peers.

2.4.5.2 Definition [WHAT?]

Trade-off decisions in an innovation process can be defined as a weighted approach involving a judgement on a wide set of criteria and is often qualitative in form, requiring a high level of expertise.

Ideally, when innovating for more safe and sustainable chemicals or processes, the new solution provides a win on all fronts. However, for complex and multidimensional assessment systems like LCA or the JRC SSbD framework, both theory and practice indicate that progress on all indicators simultaneously in real world systems will only rarely occur. The statistical probability of a solution A being better on all indicators than a solution B will decrease very rapidly as the number of assessment criteria increases.

Hence, it is somewhat unrealistic to expect a simultaneous improvement on all criteria in an SSbD innovation project. Target setting should not be about optimizing towards all criteria, but will depend on the companies' strategies in which criteria improvement is being looked for.

As visually illustrated in Figure 4, innovation is often an iterative process where (minor) steps in a supposedly wrong direction are (presently) unavoidable to take a bigger stride in the right direction, i.e. on one of the 'key indicators' or 'hotspots'.

As such, Cefic defines SSbD progress in general terms as **"a major improvement on one or more key indicators/dimensions, with no significant negatives on other relevant indicators / dimensions"**. Cefic also argues that it is not always possible or desirable to pool all indicators/dimensions into one assessment or a single score, as this may lead to results that are uninterpretable to the end user. One can argue that some dimensions exist in their own right.

Relative and absolute approaches can be considered, although the latter are typically less developed and more complex to use.

Making trade-offs in an innovation process is an evolutionary process; in the early phases the process will rely on a high degree of expert judgement, further down the innovation process more quantitative approaches can be expected.

2.4.5.3 Best practices and principles [HOW?]

There is a need for more and clearer guidance in SSbD assessment frameworks on how to deal with trade-offs. The approach should build upon common sense principles and be supported by a recommended prioritization of assessment dimensions. Suboptimal solutions or change in order of priority can be accepted in the innovation process if accompanied by a reasoned justification

a Trade-off principles – basic rules

- A priori "we would never trade off on safety". It is self-understood that safety in this context is about assessing the exposure stemming from the defined use. This being understood, we consider it good practice to assess the impact of foreseeable misuses.
- Trade-off decisions need to take a life cycle perspective.
- Trade-off decisions need to be properly documented in a verifiable way.

- Trade-off decisions are ultimately taken by those owning the innovation process. But to increase their acceptability it is recommended to discuss their foundations by experts with different fields of expertise, involving the full value chain and other actors of society.

Good practices

Trade-offs are to consider multiple criteria: e.g., hazard vs. sustainability advantages vs. performance vs. socioeconomic aspects and very often come down to a value judgment. It is considered good practice to make the rationale behind choices transparent.

Multi-criteria decision-analysis (MCDA) aims to determine the best alternative by considering more than one criterion in the selection process. MCDA explicitly evaluates multiple conflicting criteria in decision making.

Reporting on the results of an MCDA requires some fundamental choices to make in itself as well. Related to the question whether to take an absolute or relative standpoint, it should be noted that the innovation process is about incremental improvement in one or more of the safe and sustainable dimensions. It is therefore considered good practice to adopt emerging concepts such as absolute safe operating spaces to take informed decisions.

Although there are many potential approaches to come to a decision or a score in a multicriteria environment, often a 'hierarchical' approach is preferred for its transparency. The proposed JRC Framework (2022)[26] uses some a priori hierarchical elements, although it also conceptually discusses other multi-criteria decision-making approaches, which will be further explored during testing phase.

One way to get a better grip on managing trade-offs and deal with prioritization is to have an upfront and sometimes case-specific evaluation on what are the 'must-haves' and 'nice-to-haves' that define SSbD progress. For the 'must-haves' the minimum criteria should be fulfilled. For the 'nice-to-haves', it can be accepted that not all success criteria are met, or even have one or more minor negatives that in the balance will not significantly impact the acceptability of the proposed solution.

2.4.5.4 Illustrated through examples

- Enzymes in laundry detergents: Despite the fact that enzymes pose a respiratory hazard, they can offer truly unique and very significant benefits in several dimensions of the assessment scheme, e.g., stain removal at low temperature, GHG savings, etc. To manage the hazard in consumer products, enzymes are stabilized in a prill, significantly reducing the risk that the adverse effect will be expressed.
- Phosphate substitution in detergents: natural and very safe ingredient phosphate (STPP) in detergents contributed together with other P sources to undesirable eutrophication in natural waters. STPP was replaced by a combination of 2-3 other ingredients that have a somewhat higher toxicity (hazard), but can well be managed by wastewater treatment, keeping risk still very low.
- Fragrance ingredients: Fragrances typically are small molecules, which are added to many different products to improve their scent, such as perfumes, detergents and many more. New fragrances require the development of new molecules from scratch, which consequently lack rich data sets for analysis, especially during the development phase. When comparing, for example, two fragrance molecules with very different hazard profiles (one without classification, suitable for use in high concentrations like in air fresheners, and one with a hazard classification), it is crucial to also consider their potency, meaning the volume needed to reach the desired performance level as a fragrance. The risk assessment may show that the final risk of the substances is very dependent on the concentrations required for adequate performance and final application, since the hazardous substance can result in the same calculated risk as the non-hazardous substance due to the different applications and concentrations required. A full LCA cannot be performed on new substances, since sufficient quality data are typically not available.
- Cathode Active Materials (CAM) for Lithium-Ion Batteries (LIB): Lithium-ion batteries play a key role in the electrification of our mobility and therefore help avoid significant CO_2 emissions. High-performing CAMs based on transition metals (Ni, Co) oxides are hazardous (CMR) substances and could therefore be penalized in an SSbD framework. However, the industry is set up to handle those materials properly, avoiding risks for humans during production and handling (avoidance of dust formation, housing, HVAC systems, …). This is true for all steps of the process chain, including recycling. Within the battery itself, cathode active materials are safely encapsulated, and contact with consumers is avoided. Alternative CAMs like LFP (lithium iron phosphate) do not provide the necessary energy density for high-performance application segments.

3. Conclusion

3.1 Concluding remarks

To ensure a full assessment of chemical products, their contributions to applications during their use phase need to be integrated– covering the full life cycle. Our vision towards SSbD chemicals, materials, products, processes & services reflects the complexity that goes with transforming a complete industry sector at the source of the majority of industrial value chains within Europe and beyond while offering a practical and scalable solution. The following cornerstones are critical from our perspective:

- A process based on guiding principles for the innovation phase of all new products and criteria to be assessed at the level of product-application combination.
- The basic principle when innovating to improve the functionality and performance of chemicals, materials, products, or processes, is the aim to improve performance in at least one of the dimensions of safety and sustainability without significant negative impacts[27] in any of the other dimensions, compared to the incumbent solutions.
- As a minimum, a sound implementation of "Safety" shall be applied using a risk-based assessment considering the hazard, use and exposure in line with REACH and anticipating future regulatory changes. In applying SSbD, the chemical industry has the ambition to go beyond that legally fixed minimum requirement and go for continuous reduction of toxicological risks for humans and the environment based on the continuous development of knowledge around toxicological risks. This is particularly valid for consumer use and in considering the end-of-life and circularity aspects.
- The sustainability assessment[28] as an integral part of the innovation process shall cover the life cycle of a product-application-combination. All assessments shall, as a minimum cover focus dimensions deemed of high importance to reach the EU Green Deal objectives. Additional sustainability contributions may be considered.

3.2 Connect the PSA assessment framework with the assessment dimensions of an SSbD approach

PSA allows for sustainability portfolio classifications on a single product level, and is already validated and fully aligned with SSbD principles. Hence, the PSA enables a comprehensive sustainability steering on a detailed level, and a number of companies in the chemical sector are using it as a framework.

The categorisation of the portfolio is a powerful tool to support the company's innovation process to help them develop new more sustainable solutions, and address product shortcomings.

A cross-industry aligned extension of the assessment framework fitting the innovation design requirements would allow faster and effective steering towards improved products and processes with regards to "safe" and "sustainable" and is recommended to be taken forward.

4. Needs and next steps

Present guidance illustrates how in applying SSbD principles, the chemical industry has the ambition to go for continuous reduction of toxicological risks for humans and the environment especially for consumer use, additionally considering the end-of- life and circularity aspects. In order for SSbD to become a useful guidance for fast decision making, approaches must be:

- lean and pragmatic
- resource and capacity needs should be coverable by the respective existing innovation project resources.

As can be seen by the contents of this guidance, bringing in safety and sustainability considerations early into innovation processes is relying heavily on data and assessment methodologies. Hence, the development of further flexible, adaptable (digital, e.g. predictive approaches such as modelling) methodologies, analytical methods, and toolboxes, including withgoing databases, will be needed, alongside the actual target to develop new molecules, materials, products, processes and services for substitution or new approaches.

Costs will be associated with such innovations on methodologies and toolboxes. In addition, the actual development of substances is of critical nature. Given the short time left until 2050, and the complexity of investment cycles, the chemical industry needs the right funding instruments and methods, including for its academic partners.

Furthermore, data availability and accessibility along the value chain of a chemical or material plays a crucial role for the analysis throughout its entire life cycle. Here, secure approaches to data sharing and data sharing spaces need to be developed respecting the guiding principle of protection of intellectual property.

Also, to strengthen global competitiveness of the EU chemical industry and not to create a European stand-alone solution, innovation is to be considered a crucial driver and, a clear strategic link between application of any SSbD framework and the purpose of R&I innovation steering and opportunities should be pointed out, including the possibility of incentivization for industry when the assessment framework is applied (e.g. leaner registration processes).

The complementary use of any SSbD framework with established approaches, such as the PSA methodology are seen as synergistic. In going forward, we suggest to focus the application of any SSbD framework on innovation processes for future chemicals, materials, production processes, whereas established methodologies should be utilized to analyse a company's existing portfolio of chemicals, products, processes and services.

The journey to sustainability that the chemical industry has embarked on, as well as our vision for 2050, is well reflected in the vision EU policymakers have in the Chemicals Strategy for Sustainability (CSS) that "Chemicals are produced/used in a way that maximises their benefit to society while avoiding harm to the planet & people and production and use of safe and sustainable chemicals in Europe becomes a worldwide benchmark".

Cefic continues to provide input such as the present to the creation of a straightforward and "easily" applicable approach to safe and sustainable-by-design innovation between the European Commission, industry, academia and RTOs and the downstream users of the chemical sector and commits to continue facilitation of this co-creation process, bringing together all relevant stakeholders.

Annex I – Definitions

- **"Chemical":** means these substances and mixtures.
- **"Consumer and professional use":** use of the chemical/material in question in a specific product-application combination; either a) the end consumer in day-to-day life without any specific protective measures (i.e. without personal protective equipment) or b) professionals trained in the use of the chemical/material in question with a basic level of specific protective measures taken (i.e. use of personal protective equipment)
- **"Corporate requirements"** are defining the needs of the organisation undertaking the innovation. These requirements can encompass business strategies and objectives, upcoming regulation, corporate rules, stakeholder analysis results, …
- **"Hot spot"** analysis means the identification of areas to be prioritized for action concerning product portfolios, product categories or individual products.
- **"Industrial use":** use of the chemical/material in question in a specified product-application combination, here: an industrial process (chemical plant, engineering plant etc.) using state of the art measures regarding risk management and labor safety (e.g. ideally closed loop processes).
- **"Material":** a term that is used to denote either substances or mixtures which may or may not yet fulfil the definition of an article under REACH and may be of natural or synthetic origin.
- **"Materiality":** according to WBCSD PSA, signals on sustainability performance considered to be material when both of the following aspects apply:
  - › **"Significant"** - The company expects the signal to lead to changed behavior or actions by relevant stakeholders;
  - › **"Measurable"** - The signal is based on a factual observation from a credible source;
- **"Minimum requirements"** are requirements to be fulfilled at all times, e.g., regulatory requirements as enshrined in law and respecting human rights.
- **"Mixture":** means a mixture or solution composed of two or more substances.
- **"Must-have requirements"** are requirements that must be fulfilled in an innovation process good-to-have characteristics are requirements which would be beneficial to fulfill in an innovation process.
- **"Safe and Sustainable-by-Design":** At this stage, Safe and Sustainable-by-Design can be defined as a pre-market approach to chemicals that focuses on providing a function (or service), while avoiding volumes and chemical properties that may put human health or the environment at risk. Overall sustainability should be ensured by minimising the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a lifecycle perspective. [Definition taken from page 4 EU COM, CSS from Oct. 2020].
- **"Signal"** - according to WBCSD PSA, a fact-based observation on material, sustainability-related actions or commitments of key stakeholders (e.g., legislation, purchasing decisions, ecolabel requirements) that indicate whether or not stakeholders perceive the PARC as contributing to a transition to a more sustainable world. Companies identify signals through the evaluation of the public communication of key stakeholders (e.g., governments, downstream players, ecolabels, industry associations, etc.)
- **"SSbD product"** shall mean any product – including in the context of providing a service (considering the full life cycle) – which is intended for consumers or likely, under reasonably foreseeable conditions, to be used by consumers and whether new, used or reconditioned. When referring to Safe and Sustainable-by-Design products, this definition covers only the products that can also be identified as chemicals or materials (as defined above). Thus, the term 'product' in the Sustainable-by-Design context is used as part of the term "chemical product" or "material product", meaning chemicals and materials that are intended for consumers, or likely to be used by consumers. An example of a 'chemical product' is paint, and an example of a material product is 'impregnated wood'.
- **"Stakeholder requirements"** are the needs expressed by those with a vested interest in the innovation project, or whose interest may be affected by the project. Common stakeholders can be customers, consumers, investors, community, …
- **"Substance":** means 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.

Annex 2 – Authoritative and other relevant substances lists

Non-exhaustive list of elements of importance are:

- REACH authorization list (Annex XIV)
- Ban of a substance identified under REACH restrictions (Annex XVII)
- Relevant Organization for Economic Co-operation and Development (OECD) countries, which should include at least European Union, North America, China and Japan
- US 40 Code of Federal Regulations (CFR) Part 751 – Regulation of Certain Chemical Substances and Mixtures
- Laws, regulations, bans/restrictions of business relevance for a company
- Substances causing damage to the ozone layer as listed in the Montreal protocol
- Persistent Organic Pollutants (POPs), as identified under the Stockholm Convention
- Substances affecting the climate according to the Montreal- and Kyoto-Protocol
- The list of priority and priority hazardous substances of the Water Framework Directive
- Substances on the priority lists of OSPAR and HELCOM
- Substances subject to Prior Informed Consent (PIC) under the Rotterdam Convention
- Mercury-related products and processes, and control measures, as identified under the Minamata Convention
- Substances of very high concern, as identified under REACH regulation (candidate list) or similar lists in other countries
- Substances on the U.S. EPA Toxic Substances Control Act (TSCA) Work Plan for Chemical Assessments: 2014 Update
- Other lists considered to be early warning indicator, such as the EU registry of Substances of Very High Concern (SVHC) intentions or the EU registry of restriction intentions and Pool 0 substances from Restriction Road Map under EU COM Chemicals Strategy for Sustainability (CSS)
- Other relevant "opinion leading" countries (e.g., BRICS) and relevant U.S. states, such as California proposition 65 and ED List 1, administered by the Danish Environmental Protection Agency
- Pool 1 and 2 substances from Restriction Road Map under EU COM CSS
- Customer industry specific legal requirements (e.g., 1223/2009 EU Cosmetics regulation)

Notes

1 WBCSD Chemical Industry Methodology for Portfolio Sustainability Assessment (PSA) Platform - World Business Council for Sustainable Development (WBCSD)
2 https://www.undp.org/sustainable-development-goals/zero-hunger?gad_source=1&gclid=EAIaIQobChMI48vt6NG8hAMVQqeDBx1r4ALiEAAYAiAAEgIBmfD_BwE
3 Circabc (europa.eu)
4 https://research-and-innovation.ec.europa.eu/research-area/industrial-research-and-innovation/key-enabling-technologies/chemicals-and-advanced-materials/safe-and-sustainable-design_en
5 In full respect of minimum requirements, such as regulations and international conventions, which must be met.
6 It needs to be noted that work is still in progress to arrive at a mature level of sustainability assessment for many sustainability dimensions.
7 https://ec.europa.eu/environment/strategy/chemicals-strategy_nl
8 https://eur-lex.europa.eu/resource.html?uri=cellar:b828d165-1c22-11ea-8c1f-01aa75ed71a1.0002.02/DOC_1&format=PDF
9 https://ec.europa.eu/environment/strategy/zero-pollution-action-plan_nl
10 https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/europe-fit-digital-age/european-industrial-strategy_en
11 Taken from the introduction from the CSS
12 Safe and Sustainable-by-Design has been defined at this stage in the CSS as "a pre-market approach to chemicals that focuses on providing a function (or service), while avoiding volumes and chemical 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 in particular on climate change, resource use, ecosystems and biodiversity from a lifecycle perspective".
13 https://commission.europa.eu/energy-climate-change-environment/standards-tools-and-labels/products-labelling-rules-and-requirements/sustainable-products/ecodesign-sustainable-products-regulation_en
14 EUR-Lex - 32022H2510 - EN - EUR-Lex (europa.eu)
15 Strategic Research and Innovation Plan for safe and sustainable Chemicals and Materials | Research and Innovation (europa.eu)
16 The "most harmful chemicals" is a terminology introduced in the Chemicals Strategy for Sustainability under the Action "Protection against the most harmful chemicals". The Commission will a.o. extend the generic approach to risk management to ensure that consumer products –including, among other things, food contact materials, toys, childcare articles, cosmetics, detergents, furniture and textiles - do not contain chemicals that cause cancers, gene mutations, affect the reproductive or the endocrine system, or are persistent and bioaccumulative. In addition, immediately launch a comprehensive impact assessment to define the modalities and timing for extending the same generic approach, with regard to consumer products, to further harmful chemicals, including those affecting the immune, neurological or respiratory systems and chemicals toxic to a specific organ;
17 Safe and Sustainable-by-Design - cefic.org -
18 In full respect of minimum requirements, such as regulations and international conventions, which must be met.
19 It needs to be noted that work is still in progress to arrive at a mature level of sustainability assessment for many sustainability dimensions.
20 Portfolio Sustainability Assessment v2.0 - World Business Council for Sustainable Development (WBCSD)
21 Non-exhaustive list of chemical companies applying the PSA methodology as of July 2021: Arkema, Asml, BASF, Borealis, Chemours, Clariant, Covestro, Dow, DSM, Evonik, Infineum, Lanxess, Lyondellbasell, Sabic, SIKA, Solvay.
22 Cooper, R.G., 1986. Winning at new products (Vol. 26). Reading, MA: Addison-Wesley
23 EPR: Extended Producer Responsibility - EPR schemes are set up at national level in Europe and enable public authorities and producers/importers to meet obligations relating to the recycling and recovery of packaging waste.
24 Avoiding competition with food production or social or ecological land use and outweighing externalities.
25 Abiotic depletion refers to the depletion of non-living (abiotic) resources e.g. fossil fuels, minerals, clay, peat.
26 Caldeira, C., Farcal, R., Garmendia Aguirre, I., Mancini, L., Tosches, D., Amelio, A., Rasmussen, K., Rauscher, H., Riego Sintes, J. and Sala, S., Safe and sustainable-by-design chemicals and materials - 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 978-92-76-53280-4, doi:10.2760/404991, JRC128591.
27 In full respect of minimum requirements, such as regulations and international conventions, which must be met.
28 It needs to be noted that work is still in progress to arrive at a mature level of sustainability assessment for many sustainability dimensions.

Guidance endorsed by:

essenscia

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Federación Empresarial de la
Industria Química Española

Verband der
Chemischen Industrie e.V.
Wir gestalten Zukunft.
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