Atomic Layer-coated Graphene Electrode-based Micro-flexible and Structural Supercapacitors

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Executive Summary

The present report constitutes ARMS deliverable D6.1 SSbD framework report detailing criteria for safety, sustainability and circularity assessment.

This deliverable outlines a fully-fledged SSbD (Safe and Sustainable by Design) framework aimed at supporting electrochemical energy storage devices innovation across all maturity levels, from early-stage research to market deployment. The framework is designed to be publicly accessible, serving as valuable suggestions for diverse stakeholders, including 1. public research institutions engaged in fundamental and applied research on electrochemical energy storage. 2. Private sector organizations, including battery manufacturers, material suppliers, and technology developers, seeking sustainable innovation pathways. 3. Regulatory bodies and policymakers involved in shaping sustainable energy strategies.

Innovation in electrochemical energy storage is increasingly dependent on what are called Advanced Materials (AM). AM are intentionally designed and engineered to possess enhanced physicochemical properties, structural modifications, or improved functional performance to meet the demanding requirements of next-generation energy storage solutions. Nevertheless, the development of AM and their use in different product applications may present challenges including safety (in manufacturing and consumer applications), potential environmental impacts, resource dependencies, and socio-economic aspects. Given these complexities, SSbD is the recommended framework for guiding, assessing or comparing innovation avenues.

The SSbD framework elaborated in this deliverable, follows a hierarchical approach in which safety aspects are considered first, followed by environmental (including circularity) aspects, social and economic aspects. This framework prioritizes safety assessments to identify and mitigate potential hazards associated with materials, manufacturing processes, and end-use applications. This includes evaluating toxicity, occupational and environmental exposure risks. Building on this, the framework incorporates life cycle thinking to assess environmental impacts, addressing material efficiency, recyclability, and raw material dependencies. By emphasizing circularity principles, the framework aligns with broader EU sustainability goals, advocating for resource-efficient designs, secondary raw material integration, and responsible end-of-life management. Beyond environmental aspects, the framework also considers social and economic factors, such as ethical raw material sourcing, market feasibility, and alignment with just transition principles to ensure that innovation in electrochemical energy storage supports sustainability resilience.

The report also introduces a workflow for implementing SSbD in electrochemical energy storage development, integrating established safety assessment tools, life cycle modeling frameworks, and literature-based best practices. By bridging the European Commission (EC)'s overarching SSbD methodology with sector-specific sustainability challenges, this framework provides a structured yet adaptable tool for guiding responsible innovation in electrochemical energy storage technologies.

Contents

List of abbreviations

AM – Advanced Materials

CRM – Critical Raw Materials

CSS – Chemicals Strategy for Sustainability

DNEL – Derived No Effect Level

ECHA – European Chemical Agency

EFSA – European Food Safety Authority

EoL – End of Life

JRC – Joint Research Centre

LCA – Life Cycle Assessment

S-LCA – Social Life Cycle Assessment

TRL – Technology Readiness Level

MCDA – Multi Criteria Decision Analysis

NMs – Nanomaterials

NOAEL – No Observed Adverse Effect Level

OELs – Occupational Exposure Limits

PARC – Partnership for the Assessment of Risks from Chemical

PEF – Product Environmental Footprint

PNEC – Predicted No Effect Concentration

QSARs – quantitative structure-activity relationship models

REACH - Regulation on the Registration, Evaluation, Authorization and Restriction of Chemicals

SSbD – Safe and Sustainable by Design

List of figures and tables

Figures

Tables

SSbD framework for electrochemical energy storage devices

1. Introduction

With the European Green Deal (European Commission, 2019), the European Commission (EC) set concrete goals towards transforming the European Union's (EU) economy to support a more sustainable future and to implement the United Nations' agenda 2030. Among its objectives, is the Zero Pollution Ambition, manifested thorough the Chemicals Strategy for Sustainability (CSS) in 2020. Specifically, within the CSS action 2.1 - Innovating for safe and sustainable EU chemicals, sub-action 2.1.1 aims at promoting safe and sustainable by design chemicals, while the sub-action 2.1.2 aims at achieving safe products and non-toxic material cycles. In 2022, the EC adopted a Recommendation establishing a European assessment framework for 'safe and sustainable by design' chemicals and materials (hereafter SSbD). The scientific-technical basis for the framework was developed by the Joint Research Centre (JRC)(Caldeira et al., 2022a, 2022b) and later tested with concrete cases studies (Caldeira et al., 2023). The framework is currently in a period of testing. Most recently, the JRC published an updated methodological guidance to further support the testing of the framework (Abbate et al., 2024).

The EU Chemicals Strategy for Sustainability (CSS) defines SSbD as: "a pre-market approach to chemicals design 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. In this context, the overall sustainability should be ensured by minimizing the environmental footprint of chemicals in particular on climate change, resource use, ecosystems and biodiversity from a life cycle perspective". We also have the OECD definition: "the SSbD approach addresses the safety and sustainability of the material/chemical/product and associated processes along the whole life cycle, including all the steps of the research and development (R&D) phase, production, use, recycling and disposal", (OECD, 2022).

Although in the EC-CSS, the SSbD approach primarily referred to chemicals, it has been extended subsequently to include materials and products. The SSbD is proposed as a guiding framework in decision-making processes applied early in product development. SSbD approaches have been tested in the chemical sector and nano materials area for some time but are just emerging in product development and for full technology applications (Apel et al., 2024). Substantial practical challenges are acknowledged, including obtaining and generating data, and lack of maturity in tools and sustainability assessment applied at early stages of development (van der Giesen et al., 2020).

With the present deliverable, we present an adapted or customized version of the EC-CSS proposed SSbD framework, which addresses support and assessment in the development and innovation of electrochemical energy storage devices.

1.1. The SSbD framework in a nutshell

The SSbD as proposed by the EC follows a hierarchical approach in which safety aspects are considered first, followed by environmental, social and economic aspects (Caldeira et al., 2022b). The framework combines established hazard and risk assessment approaches for chemicals and materials, with sustainability assessment techniques, such as Life Cycle Assessment (LCA).

Current LCA impact assessment methodologies do assess impacts from chemical emissions from a human and environmental safety perspective (e.g., disability-adjusted life years or DALYs as an indicator), however the endpoints outlined in the EC-CSS, such as endocrine disruption, neurotoxicity, and specific organ toxicity are not specifically considered. LCA can give an indication of potential impacts, which does not reflect actual risk. Additionally, the LCA impact assessment methods are challenged by the lack of emission and toxicity data. This justifies the inclusion of specific risk assessment steps in SSbD.

The SSbD framework considers two phases:

1) **Design (or re-design) phase** in which guiding design principles are proposed to support the development of safe and sustainable chemicals and materials (such as Green Chemistry, Green Engineering, Sustainable Chemistry and Circularity), and
2) **Safety and sustainability assessment phase** in which the safety and sustainability of the chemical(s) or material(s) in question are assessed.

These two phases are iterative along the innovation process, meaning a safety and sustainability assessment should be performed since the early stages of development. The linking of SSbD assessment with the innovation process is implemented using the stage-gate model, proposed by Cooper (Cooper, 2006).

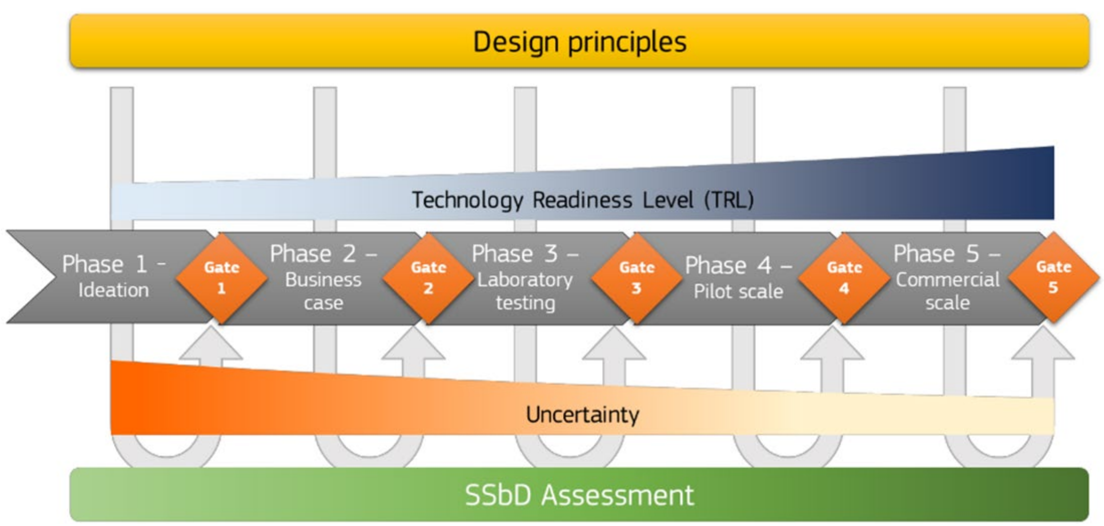

Figure 1: Linking between the innovation process phases and the SSbD assessment (figure from Caldeira et al. (2023))

The SSbD framework developed by the EC provides a general outline of a five-step assessment procedure and a set of ideas to come to an SSbD score.

The five-step approach for SSbD assessment proposed by JRC is the following:

Step 1 – Hazard Assessment

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

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

Step 4 – Environmental Sustainability Assessment

Step 5 – Socio-economic Sustainability Assessment

The last step was not included the EC recommendation and is considered optional in the framework.

1.2. SSbD toolboxes currently under development

With increased policy interest, several large EU projects are addressing SSbD, specifically the development of toolboxes to help industry and SMEs to implement SSbD assessment.

In the last decade, several European projects have aimed to develop a Safe Innovation Approach (SIA) for nanomaterials. With these projects several safe-by-design (SbD) tools were developed. The studies by Sudheshwar et al. (2024) and Salieri et al. (2021) offer overviews of tools developed in the area of nanomaterials. Some of these tools may be integrated in SSbD.

The Partnership for the Assessment of Risks from Chemicals (PARC) should be mentioned here, a 7-year partnership under Horizon Europe, consisting of more than 200 institutions working in the areas of the environment or public health from 28 countries and three EU authorities, including the European Chemical Agency (ECHA), the European Food Safety Authority (EFSA) and the European Environment Agency (EEA). One of the deliverables of PARC is an SSbD Toolbox which is still under development[1], and expected for full release sometime in 2025. The toolbox offers a comprehensive collection of tools that can be used to perform SSbD assessment, organized by innovation stage and SSbD steps (PARC, 2024).

The EU SUNSHINE project, which is nearing completion, has developed a tool infrastructure that can be used to assess materials. This infrastructure should be made public at the end of the project[2].

Many other research institutions and consultancies are also preparing assessment and decision support tools for SSbD (Braakhuis and Fransman, 2024).

[1] https://www.parc-ssbd.eu/#

[2] https://www.h2020sunshine.eu/

2. Scoping analysis for SSbD of electrochemical energy storage devices

2.1. Electrochemical energy storage

Electrochemical energy storage devices store and release energy through chemical reactions involving the movement of ions and electrons. These devices play a crucial role in renewable energy integration, grid stabilization, and portable electronics (Abbas et al., 2020).

The main types of electrochemical energy storage systems include:

1. Batteries (rechargeable) – which store energy in chemical form and convert it into electrical energy when needed
2. Supercapacitors - which store energy via electrostatic charge rather than chemical reactions, offering high power density and fast charge/discharge cycles. However, they have lower energy density than batteries.
3. Fuel Cells - generate electricity through electrochemical reactions, e.g. between hydrogen and oxygen, producing water as a byproduct.
4. Hybrid Energy Storage Systems – these combine batteries and supercapacitors or fuel cells to optimize performance.

The present framework addresses primarily rechargeable batteries and supercapacitors, as current development and innovation efforts for these devices have relatively similar goals. Electrochemical batteries are high energy density devices with typical gravimetric energy densities in the range of 75–200 Wh kg^{-1} (Abbas et al., 2020; Xu et al., 2020). Conversely, supercapacitors possess much lower energy densities, with commercial electric double layer capacitors having energy densities are in the range of 5–10 Wh kg^{-1} (Dong et al., 2023). Supercapacitors have high power density, fast charge/discharge cycles, and longer cycle life compared to batteries, but also suffer higher self-discharge rates in some cases. Figure 2 illustrates energy density vs. power density for currently commercial electrochemical energy storage technologies.

The goals of innovation for batteries and supercapacitors generally are to:

- Increase energy/power densities coupled with increasing fast charge/discharge rates, operational safety, and high cyclability.
- Substitution of materials such CRMs, or materials that have issues with high costs, safety concerns (e.g., lithium), or high environmental and/or social impacts (e.g., cobalt).

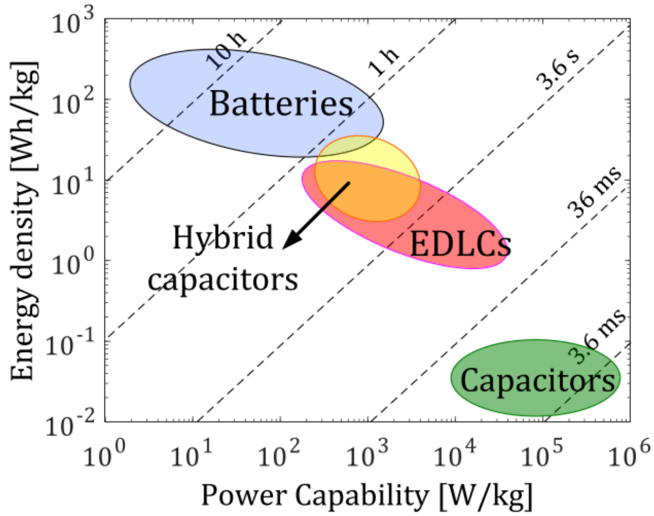

Figure 2: Ragone plot illustrates the energy density vs. power density of electrochemical energy storage technologies (commercial devices and laboratory proto-type cells that are fully packaged). (Zhao and Burke, 2021).

2.2. The use of new and advanced materials in energy storage devices

Innovation in electrochemical energy storage is increasingly dependent on what are called Advanced Materials (AM). AM are intentionally designed and engineered materials to have enhanced properties, targeted or enhanced structural features with the objective to achieve specific or improved functional performance[3].

In 2024, the EC released a communication on AM for Industrial Leadership (European Commission, 2024), which recognizes the need for Europe to focus efforts in this area. Advanced materials are hey enablers for innovation supporting the Green & the Digital Transition, with applications across many sectors, e.g. for renewable energy, batteries, zero-emission buildings, semiconductors. AM have potential to substitute certain Critical Raw Materials (CRMs) of which the EU is mostly import dependent. The EC communication also places SSbD at the core of the material transformation process, stating that development has to shift to "advanced materials that contribute to safety and sustainability, while at the same time being cheaper and performing better under all environments".

Some categories of multi-component nanomaterials (MCNMs) can be considered Advanced Materials. MCNM may be described as materials that consist of two or more functional components (e.g., nanoparticles, organic molecules, etc.) conjugated by strong molecular bonds, or formed by a nano-material (NM) with a unique chemical origin modified by hard or soft coatings (Pizzol et al., 2023). Some of the most widely used components are (combinations of) carbonaceous (e.g., fullerenes, carbon nanotubes, graphene) or metallic (metal or metal oxide) NMs with or without organic coatings (e.g., polymers, macromolecules and enzymes). MCNMs can offer significant technological benefits as the

[3] OECD working description on advanced materials https://one.oecd.org/document/ENV/CBC/MONO(2022)29/en/pdf

integration of different components in a unique system can produce new or improved functionalities. However, MCNMs can also pose substantial design challenges as well as environmental, health and safety concerns (Furxhi et al., 2023).

Based on Hong et al. (2023), a nano-enabled product (NEP) contains nanomaterials or nano-enabled materials (i.e., powders, suspensions, composites or membranes incorporating nanoscale structures, such as nano-thin layers or nanoporous matrixes). Nanomaterials can remain integrated into NEPs after their manufacturing process or may not appear in the final product (e.g., a nanocatalyst used in biodiesel manufacturing). The latter is termed nano-enabled manufacturing.

Key technical concepts in many innovation avenues for batteries and supercapacitors (including the present ARMS project) include nano-enabled materials, such as to develop highly capacitive supercapacitors by modifying graphene-rich electrodes with ultrathin (nm scale) conformal coatings via atomic layer deposition (ALD) processes.

2.3. Definition of the system under study

To perform an SSbD assessment, the system studied, and the innovation goal have to be defined. This includes the identification of the chemicals/materials which are at the core of the development and innovation process, the processes by which they are manufactured, and the final product and potential applications. The system definition can point to potential hotspots along the lifecycle of the product, and trigger innovation adjustment/iterations and/or the comparison of alternatives.

Innovation for electrochemical devices is driven by functional performance. Important functionality parameters include energy efficiency, power density and energy density, cycle life and shelf life, and electrolyte/electrode degradation. It is important to consider that performance parameters may influence each other and thus may also indirectly influence the safety and sustainability of devices.

The goal of innovation should include the use of design principles. The JRC SSbD framework for guidance proposes generic design principles which can be expanded according to the needs of the specific sector under consideration and the particular application under study.

Table 1: Summary of design principles (Caldeira et al., 2022b)

SSbD principle (based on)	Definition	Examples of indicators
SSbD1 Material efficiency	Incorporation of all the chemicals/materials used in a process into the final product or full recovery inside the process, thereby reducing the use of raw materials and the generation of waste.	• Net mass of materials consumed (kg/kg) • Recycling efficiency/recovery rate (%) • Total amount of waste (kg/kg) • Critical Raw Material presence (yes/no)
SSbD2 Minimize the use of hazardous chemicals/ materials	Preserve functionality of products while reducing or completely avoid using hazardous chemicals/materials where possible	• Biodegradability of manufactured chemical/material • Classification of raw chemicals/materials as SVHC[4] (yes/no)
SSbD3 Design for energy efficiency	Minimize the overall energy used to produce a chemical/material in the	• Energy consumption (kWh/kg or MJ/kg)

[4] The European Chemical Agency (ECHA) substances identified as Substances of Very High Concern (SVHC)

	manufacturing process and/or along the supply chain.	• Energy efficiency (%)
SSbD4 Use renewable sources	Target resource conservation, either via resource closed loops or using renewable material/ secondary material and energy sources	• Renewable or fossil feedstock? (yes/no) • Recycled content (%)
SSbD5 Prevent and avoid hazardous emissions	Apply technologies to minimize and/or to avoid hazardous emissions or pollutants in the environment.	• Wastewater to treatment (m3/kg) • Amount of hazardous waste (kg/kg)
SSbD6 Reduce exposure to hazardous substances	Eliminate exposure to chemical hazards from processes as much as possible. Substances which require a high degree of risk management should not be used and the best technology should be used to avoid exposure along all the life cycle stages	• Biodegradability of manufactured chemical/material • Classification of raw chemicals/materials as SVHC (yes/no)
SSbD7 Design for end-of-life	Design chemicals/materials in a way that, once they have fulfilled their function, they break down into products that do not pose any risk to the environment/humans. Design for preventing the hindrance of reuse, waste collection, sorting and recycling/upcycling.	• Recyclable? (yes/no) • Durability (years) • Disassembly/reparability design (yes/no)
SSbD8 Consider the whole life cycle	Apply all design principles throughout the entire lifecycle, from supply chains of raw materials to end-of-life	• Material Circularity Indicator (MCI)
Other, based on specific sector under consideration and the particular application		

Important boundary conditions in setting the goals of innovation are also determined by the existing legislation in the specific sector or product application.

Batteries are covered by specific legislation in the EU, specifically Regulation (EU) 2023/1542 concerning batteries and waste batteries (European Parliament and the Council of the European Union, 2023). Which replaced former Directives. The new regulation emphasizes safety and sustainability, setting targets for collection of waste batteries, lithium recovery targets, recycling efficiency targets, as well as mandatory levels of recycled content of several materials in manufacturing of new batteries.

Regarding supercapacitors, the above regulation may cover pseudo capacitors which fit under the definition for “battery” but not carbon double layer super capacitors.

2.4. Definition of the boundaries of the assessment

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

In Figure 3 below, we illustrate in the form of a diagram the generic lifecycle steps of electrochemical energy storage devices and denote by surrounding colored boxes the scope of assessment for the steps of SSbD.

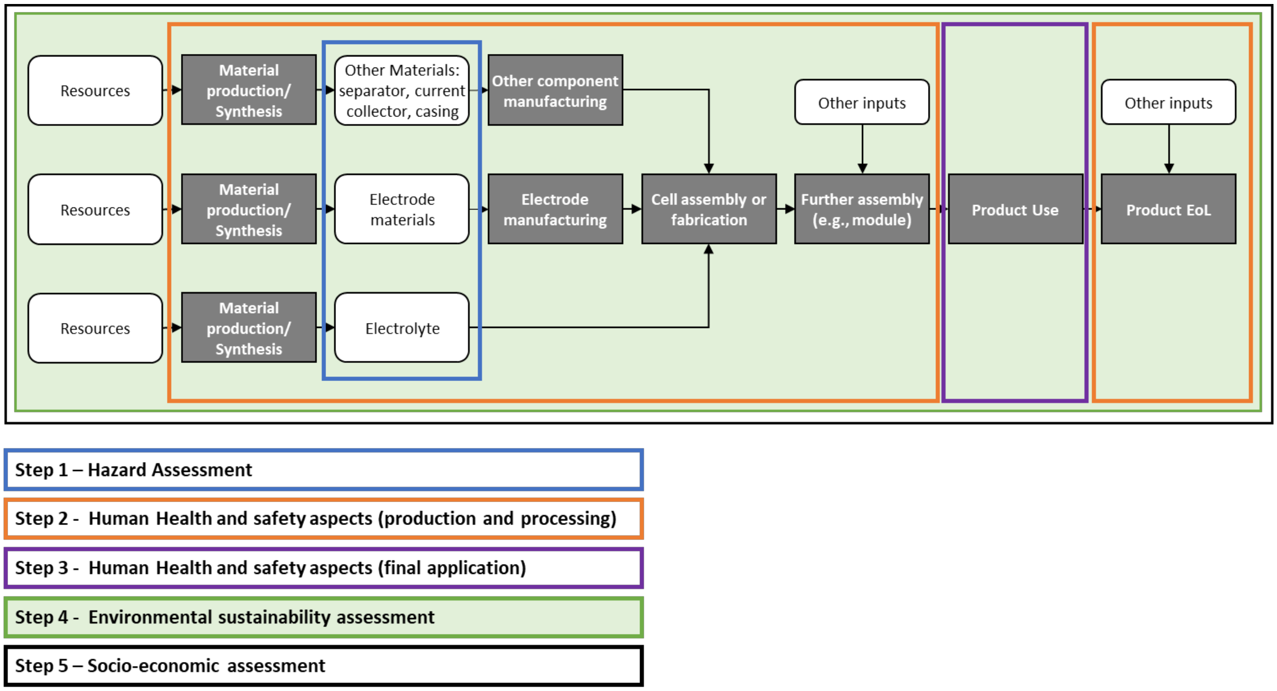

Figure 3: Product lifecycle for electrochemical energy storage devices and the scope of individual steps of the SSbD assessment.

2.5. Iterative and tiered approach for the SSbD assessment

The SSbD framework follows the iterative nature of any innovation. Hence, several iterations of the SSbD assessment are carried out along the innovation.

The iterations are generally linked to increasing knowledge of the innovation (i.e., data) and thus SSbD is implemented following a tiered approach (illustrated also in Figure 1). The tiered approach can follow the Technology Readiness Level (TRL) of the innovation to go from a simpler to a more complete version. The proposed framework for electrochemical energy storage follows largely the methodological guidance from the EC (Abbate et al., 2024). An overview of the tiered approach is given the Table 2 and detailed description follow in subsequent chapters.

Table 2: Description of tiered approach of the SSbD assessment

	Simplified **TRL 1-3**	**Intermediate** **TRL 4-7**	**Full** **TRL 8-9**
Description	Screening assessment guided by the goal of innovation	Simplified version of the SSbD	Complete and full version of the SSbD assessment
Steps 1-3: Safety Assessment	Screening approach to refine/ filter innovation if red flags are raised by: • Physico-chemical and fate properties that might raise exposure concerns • Hazard profile potential due to similar structures and structural alerts • Relevant hazard properties for the identified applications. **Sources or tools:** Generic information on chemicals/materials and uses can be retrieved from extended Safety Data Sheets.	The scope is expanded to cover all the aspects in a tiered Risk Assessment approach and as data becomes available. This includes both Hazard and Exposure assessment. **Sources or tools:** Generic information from extended Safety Data Sheets. Prediction tools such as the options listed in the PARC Toolbox	Full Risk Assessment considering the entire life cycle.
Step 4: Environmental Sustainability Assessment	Narrowed system under study, representing the stages of the life cycle that are directly affected by the goal of innovation. **Sources or tools:** Simplified tools for data generation, or process simulation	Streamlined LCA cradle-to-gate or cradle-to-grave. The Life Cycle Inventory requires collection of primary data from the actors along the lifecycle. Secondary data is used to fill gaps.	Full LCA recommended to be performed following the PEF/ Environmental Footprint method. Additional recommendations include consequential modelling of markets, and the inclusion of prospective modelling approaches.
Step 5: Socio-economic Assessment		Simplified Social LCA (S-LCA) and Life Cycle Costing (LCC)	Social LCA (S-LCA) and Life Cycle Costing (LCC), Levelized Cost of Storage (LCOS)

3. Safety assessment

This section gives an overview of Steps 1 to 3 in the SSbD framework:

Step 1 - Hazard assessment

- Hazard identification for the chemicals/materials part of the development and innovation
- Hazard characterization: the derivation of maximum exposure limits.

Step 2 and 3 – Safety aspects production, processing, final application, and EoL

- Exposure identification and assessment (for humans and environment)
- Risk characterization

In steps 2 and 3 the goal is to combine hazard with potential for exposure to determine actual risk.

3.1. Step 1: Hazard Assessment

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

The hazard assessment can be further broken in three activities:

1. Data collection, evaluation and integration
2. Hazard classification
3. Hazard characterization

Data collection, evaluation and integration

If the assessment targets a product (e.g., battery cell or supercapacitor) rather that a specific new material, the first step must be making an inventory of the chemicals and materials used in the product.

The next step is to gather all available and relevant data with regards to the physicochemical, toxicological and ecotoxicological properties for the inventoried chemicals and materials. The reliability, relevance, and adequacy of the available information must be considered. In a final step, data gaps should be identified and a strategy to generate further data can be developed. This is dependent on the goal of the assessment and the maturity of the innovation (i.e., TRL level).

Existing materials and chemicals that are placed on the European market (above one tonne per manufacturer/imported per year), have to fulfill regulatory requirements (e.g., REACH, CLP[5]). Therefore, information on the intrinsic properties of the chemicals that have been used to conclude on the hazard classification should be available in the database of the European Chemicals Agency (ECHA).

If data is not available or very scarce, such as for new materials at early innovation stages, new approach methodologies (NAMs) can be used, such as in silico models and tools (e.g. quantitative structure– activity

[5] Classification, Labelling and Packaging (CLP) Regulation ((EC) No 1272/2008).

relationship models (QSARs)), or in vitro tests, if possible to conduct. For material mixtures, or complex substances, it is suggested to take a substance component approach when using in silico models.

Hazard classification

The CLP hazard classes and categories are split in the three groups introduced in the CSS: most harmful substances (H1), Substances of concern (H2) and other hazard classes (H3) (Caldeira et al., 2022b).

From a design perspective, chemicals and materials which do not pass the Criterion H1 in Step 1 should be prioritized for substitution or redesigned to reduce adverse effects, or can be allowed if the use is essential for society (e.g., if their use is necessary for health, safety or is critical for the functioning of society and if there are no alternatives). In the latter case, emissions/exposure must be controlled along the whole life cycle.

Hazard assessment

The information collected or generated at previous steps is used to derive the tolerable maximum level of exposure for the assessment in the following Steps 2 and 3 of the SSbD framework.

The following indicators can be used:

- Derived No Effect Level (DNEL) and the No Observed Adverse Effect Level (NOAEL), which are the maximum levels above which a particular human population (e.g. workers, consumers) should not be exposed
- Occupational Exposure Limits (OELs) are other types of maximum levels above which, in this case, workers should not be exposed
- Predicted No Effect Concentration (PNEC) is the maximum concentration of a substance above which a particular environmental compartment (e.g. soil, water, air) should not be exposed.

The study by Soeteman-Hernández et al. (2023) can be mentioned here. The authors used indicators such as PNEC and NOEL to evaluate and compare 22 different types of battery chemistries. This served as a simplified safety assessment.

3.2. Step 2 and Step 3: Safety aspects in production, processing and final application

Activities for which there is a potential for human or environmental exposure to a chemical/material are defined under REACH (European Parliament and the Council of the European Union, 2006) as "use" and include processing, formulation, consumption, storage, keeping, treatment, filling into containers, transfer from one container to another, mixing, and production of an article or any other utilization.

The EC SSbD distinguishes uses that are industrial (production and processing) and final application use (by consumers or users of the product final application, such as a battery or supercapacitor).

The present section gives an overview of Steps 2 and 3 in SSbD:

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

Safety or risk assessment consists of the hazard assessment (linking to Step 1), the exposure assessment (identification of use and prediction of exposure), and the risk characterization (the estimation of the severity of the effects due to exposure).

Exposure identification and mapping

The basis for the exposure assessment is exposure scenarios. The development of the exposure scenarios starts with the mapping of the uses situation along the lifecycle of the innovation under assessment, including final product use and EoL.

The EC SSbD methodological guidance details the steps for identification of exposure scenarios (Abbate et al., 2024). Exposure scenarios can include several contributing scenarios. A contributing scenario describes each contributing activity within an identified use, for example mixing, transferring into small containers, or applying a substance or mixture by spraying.

The uses are described by The REACH use descriptor, a system developed by ECHA to facilitate chemical risk assessment and supply chain communication. Besides describing the use, the operational conditions in which these uses take place need to be considered for the exposure estimation. This includes risk management measures (RMM) and operational conditions, for which ECHA provides guidance.

The identification of the exposure scenarios, together with the description of the operational conditions/use conditions, provide the information to predict the exposure potential that can be minimized to ensure safe use by applying risk management measures. For predefined scenarios, exposure databases are employed for this task.

Data sources that can be used:

- Safety Data Sheets, that are a globally recognized tool and are widely used for communicating information on chemicals and materials. They are also an integral part of REACH in the EU.
- Use Maps - give an overview of the common uses in a specific sector using the REACH use descriptor system.
- RMM libraries, such as the one set up by CEFIC (European Chemical Industry Council).

The organization ECHA provides a Use Map Library[6], which contains map developed for different sectors and map templates that can be used to develop maps for sectors not yet included. At the moment, a map for energy storage devices does not exist.

If no predefined scenario is available or the operational/use conditions are special, exposure can be estimated using models such as the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC), Targeted Risk Assessment (TRA) and European Union System for the Evaluation of Substances (EUSES) and are used as input parameters to derive exposure estimates.

Risk Characterization/assessment

In this phase, known exposures and/or the predicted exposure are compared with the available toxicological knowledge from the hazard assessment (Step 1) in a risk characterization. If the available

[6] https://echa.europa.eu/csr-es-roadmap/use-maps/use-maps-library

data indicate that for certain uses the risk is too high, e.g. the allowed DNEL/NOAEL values are exceeded, further refinement may be needed for the exposure assessment.

At the product level, released chemicals may also imply safety risks to humans that are exposed to them. Examples of safety issues during operation include the fire/explosion hazard of lithium-air batteries or the thermal stability issues may lead to combustion, fire or explosion risks in lithium-iodine batteries (Willstrand et al., 2023). Several testing standards exist for both batteries and supercapacitors exist, including for example flammability, impacts and puncture testing.

3.3. Workflow Steps 1-3 example toolbox

The following example shows a model pipeline based on the PARC toolbox that is largely suitable for energy storage innovations with different levels of maturity.

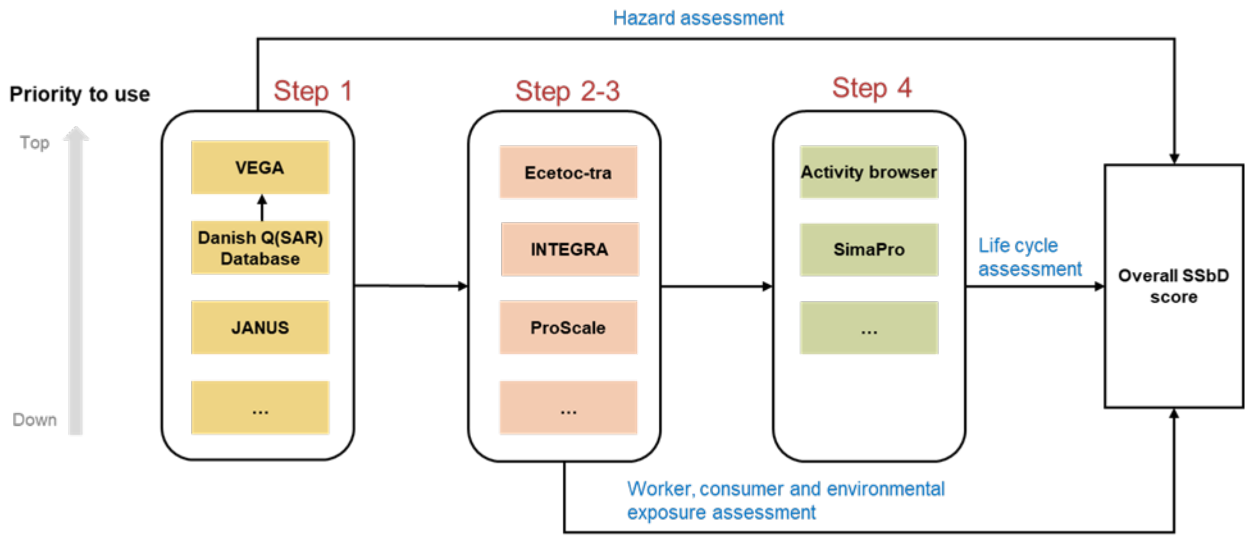

Figure 4: Pipeline of available tools for SSbD assessment

Step 1 – Hazard assessment

There are a couple of tools available for the first step. For instance, VEGA is a freely available software, developed by Istituto di Ricerche Farmacologiche Mario Negri (IRFMN), which provides over 100 QSAR models for predicting physico-chemical and (eco)toxicological properties of chemical substances. The QSAR models in VEGA are based on other tools, including EPI Suite, Toxtree, CAESAR, and SARpy. The QSAR models are built on three fundamental components, which are the property under investigation, the chemical data and the algorithm connecting the two. VEGA combines the QSAR models with read-across tools for the evaluation of the substances, providing qualitative/quantitative toxicity results and their reliability[7]. See Figure 5 the general steps to execute hazard assessment using VEGA.

[7] VEGA HUB - VEGA interpretation, available: https://www.vegahub.eu/download/vegainterpretation

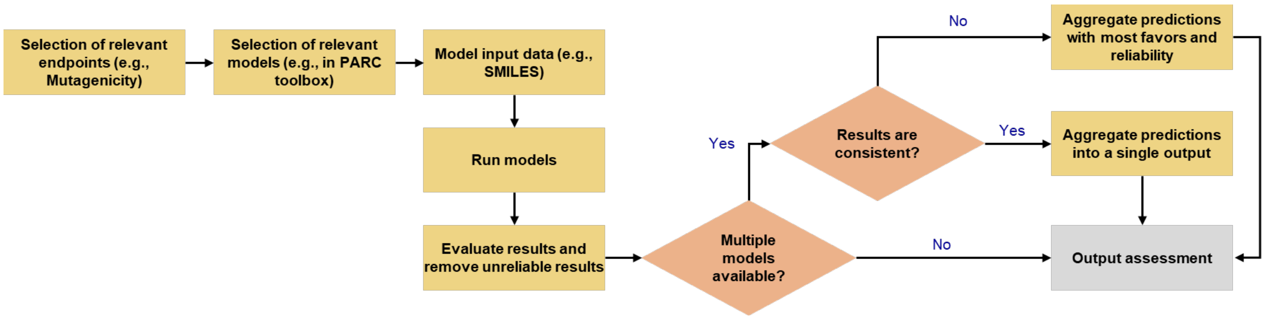

Figure 5: Steps to conduct hazard assessment (taking VEGA as an example).

Step 2 and 3 – Safety aspects in production, processing and final application

In second and third step, Targeted Risk Assessment tool (ECETOC-TRA) is a free tool developed by the European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC) to help estimate the risk of chemical exposure for workers, consumers, and the environment. This tool considers different exposure scenarios, and it can provide occupational and consumer exposure and risk estimates for inhalation, dermal and oral exposure routes. It is a user-friendly designed tool that can be used for screening assessment and is integrated into the Chesar (Chemical Safety Assessment and Reporting) tool as part of the occupational and consumer exposure assessment (ECETOC, 2012). See Figure 6 the general steps to execute human and environmental exposure assessment using ECETOC-TRA.

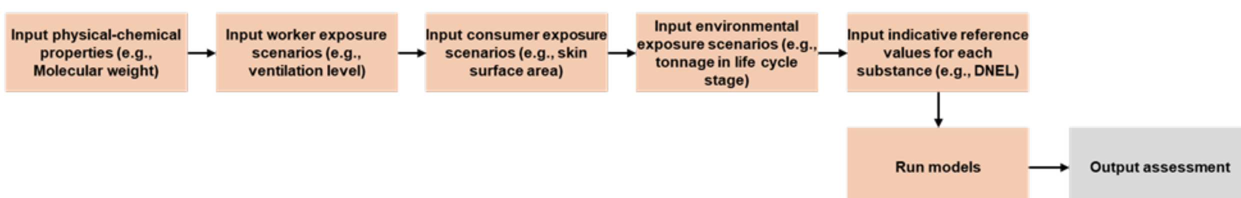

Figure 6: Steps to proceed human and environmental exposure assessment (taking Ecetoc-tra as an example).

4. Environmental sustainability assessment

Environmental sustainability assessment is performed by Life Cycle Assessment (LCA). This section covers the tiered approach to LCA taking into consideration the maturity of innovation (i.e., TRL). This means that the LCA is progressively refined over iterations, as the innovation or technology matures. LCA methodological aspects are detailed considering the tiered approach in the SSbD framework.

As defined in the ISO standards, the section will cover the four steps of LCA: goal and scope definition, life cycle inventory, life cycle impact assessment, and results interpretation. We include in the current framework also an assessment of circularity potential and material criticality as part of the environmental sustainability assessment.

4.1. General methodological considerations for LCA

Life Cycle Assessment (LCA) is a systematic method for evaluating the environmental impacts of a product, process, or service throughout its entire life cycle. The overarching method principles for conducting LCA are described in the international standards ISO 14040 (2006) and ISO 14044 (2006).

The EC SSbD methodological guideline recommends that the LCA methodology for medium to high TRL is the Product Environmental Footprint (PEF) method (European Commission, 2021; Zampori and Pant, 2019). The PEF method is based on the ISO standards, but with considerable changes. It can be stated that the PEF method is still subject to development. In relation to energy storage, Product Environmental Footprint Category Rules (PEFCR) based on the PEF method are under revision for batteries and accumulators.

Energy storage technologies, devices, and products, play a critical role in the Green & the Digital Transitions by enabling renewable energy integration and improving energy efficiency. Consequently, they have the potential to drive large-scale transformations in energy infrastructure, industrial processes, and economic systems. It is essential that the Sustainable-by-Design framework reflects these broader systemic impacts. Here, we introduce the consideration of different LCA modelling frameworks and their appropriate application.

Within LCA there are two main modelling frameworks, which can be chosen depending on the decision-making context (EC-JRC, 2010). An attributional framework is generally recommended for micro-scale decision context, while the consequential framework for meso- or macro-scale. The scale is defined by the potential of the system under study to affect the surrounding large scale societal systems (e.g., energy production, transport). Even though the system assessed may be a specific product (e.g., a new supercapacitor technology), the potential wide uptake of that product (over incumbent products) may have large scale effects, such as changing the makeup of current technology markets. These effects are not captured by the attributional approach.

One of main modelling difference between the two frameworks is the use of average data (attributional) vs. marginal data (consequential). Average data (e.g. the electricity market mix in a year) denotes a static, accounting perspective, while marginal data, which involves identifying market players that will react to the decision taken, denotes a more future oriented perspective.

The PEF method follows largely an attributional approach, although it includes elements of consequential modeling. The Circular Footprint Formula (CFF) models EoL processes, such as recycling by substitution, a modelling technique that is often associated with consequential LCA (Schrijvers et al., 2021).

4.2. Goal and Scope Definition

The goal of an LCA is generally to compare systems or products and provide decision support in regard to environmental sustainability aspects of choosing between the compared systems.

The scope of the assessment entails the definition of a Functional Unit, systems boundaries, as well as geographical and temporal boundaries. The choice for LCA Impact Assessment Method is generally also given in this phase.

To conclude on the methodological considerations presented in the previous section, we recommend the following for the overall LCA method approach:

- At low TRL, which generally allows only for simplified assessment approaches, limited scope LCA should be performed following the general PEF method approach or Carbon Footprint methods, such as specified in ISO 14067 (2018).
- At medium and high TRL, the overall LCA method approach should be determined by goal of the innovation and the potential for large scale effects. In all cases, the EC recommended PEF method can be followed as a base. This is particularly fine for innovations that target specialized applications that have only limited uptake potential. For innovations with wide uptake potential, we recommend performing the LCA based with the consequential approach.
- At medium and high TRL, the temporal scale (timeline) between the start of the innovation and the placing of the end-product of the innovation process on the market, should be considered.

Functional Unit

The Functional Unit (FU) defines the qualitative and quantitative aspects of the function(s) and/or service(s) provided by the product being evaluated. For system/product comparisons, the FU is used as reference unit and must be identical for the compared systems.

For electrochemical energy storage the definition of FU given in the recent EU batteries regulation is quite appropriate, respectively: ''The functional unit is further defined as one kWh (kilowatt-hour) of the total energy provided over the service life by the battery system, measured in kWh. The total energy is obtained from the number of cycles multiplied by the amount of delivered energy over each cycle.''

The importance of using the right FU in LCA of batteries has been covered by scientific reviews such as by Porzio and Scown (2021).

System boundary

For low TRL innovations, where only a simplified assessment can be performed, Cradle-to-Gate system boundaries are appropriate id potential (product) applications are not yet well defined. At higher TRL levels, where streamlined of full LCA can be performed, the system boundaries should be Cradle-to-Grave, i.e., the use and EoL lifecycle stages are included. The system boundary for the environmental assessment is illustrated in Figure 3.

Selection of the reference/ benchmark

The selection of appropriate reference/benchmark is dependent on the goal and level of innovation. As previously stated, LCA is performed with the goal to compare systems. The reference/benchmark is a material, a process, or a product that provides the same function or service (quantified by FU) as the new (the innovation) material, process, or product. These are materials, processes, or products that exist on the market today (e.g., commercially available supercapacitors). Ultimately the goal of SSbD is to determine and ensure that an innovation can provide the same function but with higher safety and lower environmental impacts.

4.3. Life Cycle Inventory: Data generation and collection

The life cycle inventory (LCI) involves data collection and quantification of all inputs (resources, energy, and materials) and outputs (emissions, waste, and products) associated with a product, process, or service throughout its entire life cycle.

The LCI is typically process-based, relying on measured or modeled data for processes (or activities) at each stage of the product's life cycle (e.g., raw material extraction, manufacturing, use, and end-of-life disposal). LCI blocks define data blocks pertaining to unit processes. Unit processes have to be defined at a technology-wise appropriate level of aggregation (e.g., component level). Unit processes are defined in the ISO standard as the "smallest element considered in the LCI analysis for which input and output data are quantified".

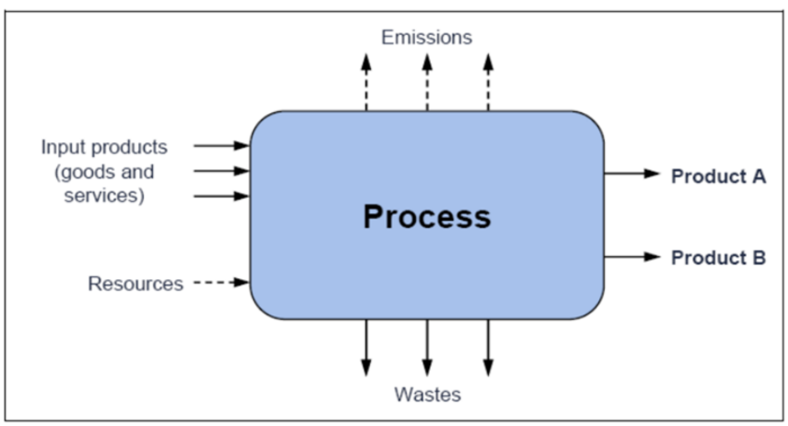

Figure 7: Illustration of a unit process, showing the various measure or modelled data flows (EC-JRC, 2010)

Guidance for generating the LCI is provided by the PEF method. Additionally, systematic approaches and stepwise guidance for data collection in the life cycle inventory have been elaborated, see for example Kellens et al., (2012) and Saavedra-Rubio et al. (2022).

From a data point of view, it is useful and also a part of the PEF approach to split a system into a foreground and background systems. The part of the system directly describing or addressing the innovative process/es is considered the foreground, while the upstream and downstream processes to the foreground are referred to as the background system. Data for background systems is compiled from LCI databases (e.g., ecoinvent).

The LCI of the innovative technology under assessment (i.e. the foreground system) is iteratively updated throughout the innovation process. At low and medium TRL levels, the process data available may be severely limited and may be based on laboratory or pilot scale processes. However, the comparison against reference/benchmark technologies requires that the innovative technology also be represented at industrial scale. The EC SSbD framework methodological guidance makes suggestions for how this may be achieved.

Industrial scale may be represented by generating data with process simulation tools (e.g., Aspen Plus). Furthermore, read-across principles that are applicable for chemicals can be applied as well to processes. For unknown processes, known processes likely to have similar conditions (inputs, equipment, emissions) can serve as proxies. Further technology upscaling methods, based on learning curves and scenario approaches, are also proposed (Tsoy et al., 2020).

Finally, at medium and high TRL, the temporal scale (timeline) between the start of the innovation and the placing of the end-product of the innovation process on the market, should be considered in the LCI. Future uptake and use scenarios for the technology should be considered under consequential LCA modelling. Under these conditions, the background inventories should reflect or include foreseen future changes of external aspects (e.g. changes in the electricity provision). To achieve this, new tools for modifying background inventories based on future scenarios have been developed (Sacchi et al., 2022).

4.4. Life Cycle Impact Assessment (LCIA)

Impact assessment is the LCA phase where the potential environmental impacts are derived based on a number generally standard methodologies which associate characterization factors (and later normalization factors) to all process exchanges with the environment which are described in the LCI.

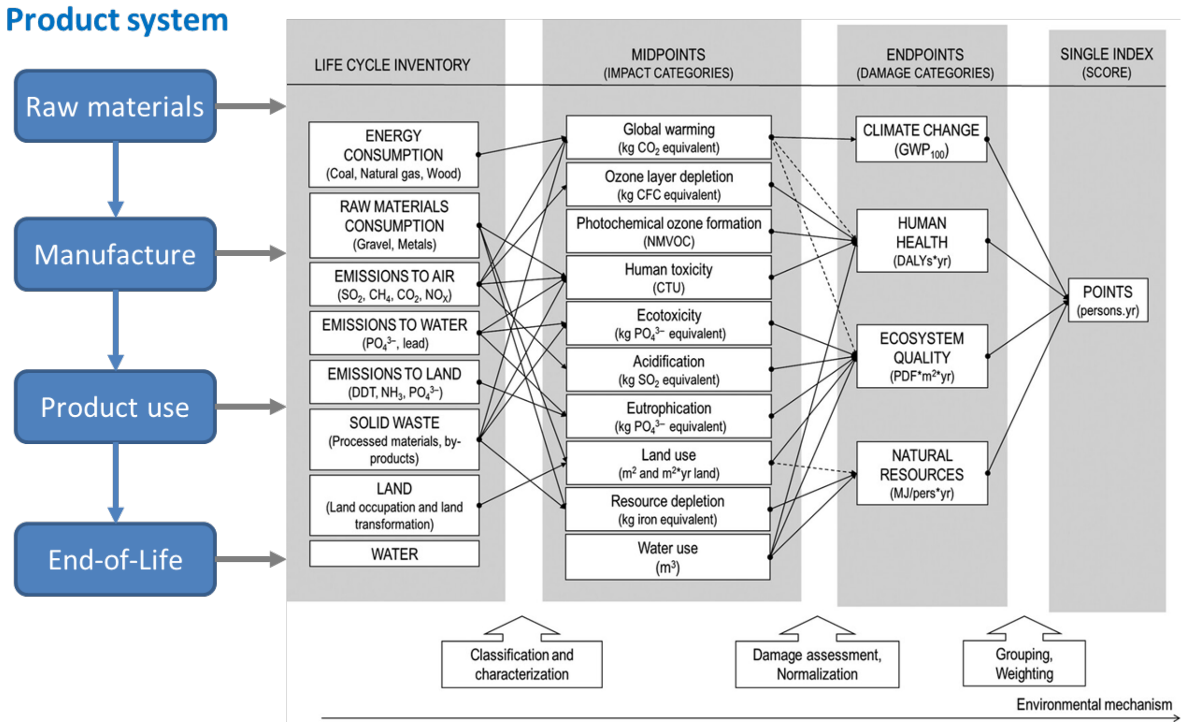

Figure 8: Representation (simplified) of the mechanisms behind impact assessment, from inventory data (example of elementary flows) to final results (given in a single score), including midpoints and endpoints. CTU, Comparative Toxic Unit; NMVOC, Nonmethane Volatile Organic Compound; GWP100, Global Warming Potential (time horizon of 100 years) DALY, Disability Adjusted Life Years; PDF, Potentially Disappeared Fraction of Species. The figure is by own elaboration including base diagram from Souza et al. (2015).

The SSbD framework recommends the use of the Environmental Footprint (EF) method which has been developed for PEF.

For high TRL, the inclusion in the full LCA of the Absolute Environmental Sustainability Assessment approach could also be relevant.

The EC SSbD framework considers the use of absolute sustainability assessment methods, as they would allow to consider ecosystems carrying capacities in environmental assessments. In recent years, several methods have been developed linking the Planetary Boundaries (PB) framework to LCA. Normalization references that can be applied to characterized results from the EF method have been developed (Sala et al., 2020).

4.5. Interpretation of LCA results and links to the (re)design

Elements of interpretation are connected to all previous steps of LCA but particularly in connection to assessment results. Generally, the objective is to understand the quality of the model (e.g., by considering uncertainty), and to understand the processes or elementary flows that have high contribution to different impacts (i.e., so called contribution analysis).

For energy storage devices, this step helps pinpoint critical hotspots across the life cycle. For instance, environmental hotspots in supercapacitors may arise from the production of high-purity activated carbon or graphene, which requires energy-intensive processes such as chemical activation. Identifying these hotspots provides valuable feedback for prioritizing (re)design strategies (Luanwuthi et al., 2024).

4.6. Assessment of circularity and material criticality

"Sustainable by design" overlaps to some extent with other concepts, such as "eco-design" and more recently with "circular by design". All these connect products with sustainability, which can be analyzed with life cycle thinking approaches (Apel et al., 2024; Sudheshwar et al., 2024). Thus, assessment of material efficiency indicators is important in SSbD.

Circularity assessment

The Circularity assessment should align with existing EU policies, particularly the recently adopted Battery Regulation. The Regulation mandates targets for waste batteries collection (e.g., 73 % by 2030 for portable batteries), lithium recovery, recycling efficiency (e.g., 70 % by 2030 for lithium-based batteries), as well as minimum levels of recycled content in new batteries. While primarily focused on batteries, these regulations are highly relevant for all electrochemical energy storage devices.

A large variety of circularity indicators have been developed over the last decade, with many following complex approaches that can be difficult to apply to new products and applications (Corona et al., 2019; Kristensen and Mosgaard, 2020). At early stages of the innovation process, data on the fate of materials and products is largely absent. The consideration of circularity is highly relevant at middle stages in the innovation process, where (re)design can have a large influence on circularity outcomes.

A comprehensive circularity assessment follows a lifecycle system approach, such as the overall environmental sustainability assessment. The following elements should be considered and evaluated if possible:

- Source of resources used – recycled input content and content/feedstocks from renewable sources.
- Resource efficiency in production – how much (i.e., ratio) of materials used are incorporated into the product vs. becoming production scrap.
- Design for reuse and/or recycling – the product ca be reused in similar of different applications, the products components and materials can be separated/disassembled.
- EoL management systems – to what extent infrastructure for recovery/collection and processing/recycling already exists for the materials/products developed.

A number of recycling technologies and approaches exist for electrochemical energy storage devices: from direct reuse (in potentially different applications than the original), pyrometallurgical and hydrometallurgical pathways, and combination mechanical recycling approaches with pyro- or hydro metallurgy (Di Persio et al., 2024; Xu et al., 2020). The innovative goal or the product application, should be evaluated for compatibility with existing recycling routes. If the innovation/products are not compatible with existing recycling or may be dependent on developing highly dedicated recycling techniques, (re)design options can be considered. However, potential environmental benefits of increased circularity should be weighed against overall environmental gains of the innovation. For example, if redesign for circularity impacts the lifetime of functional goal of the innovation, which results in significantly loss of environmental benefits, the design for circularity should be less prioritized.

Different indicators can be used to compare a product against a reference or benchmark. In Table 3, a selection of three indicators that address the material and product level is proposed. Nevertheless, these indicators do not capture all the dimensions listed previously in the section. It is therefore recommended that several indicators are used together (Moraga et al., 2019).

In the absence of detailed data for the calculation of indicators, other simplified tools may be useful to guide the innovation process. A circularity scorecard (in questionnaire form) may require only expert input to evaluate broadly if there are substantial hotspots in relation to circularity of a products under development. Results can be aggregated in the simplest form by summing "yes" and "no" answers to a set of criteria, such as in the example by scorecard in Cimpan et al. (2023).

Table 3: Circularity indicators at material and product-level

Indicator	Description	Source
Material Circularity Indicator (MCI)	The MCI considers the recycled con- tent in a product along with waste (linear flow) and utility of a product (expressed through lifetime).	(Ellen Macarthur Foundation and ANSYS Granta, 2019)
Product-level Circularity Metric (PLCM)	PLCM uses the economic value of recirculated parts (recycled and refurbished) and the economic value of all parts to calculate product circularity, which is defined as the fraction of a product that comes from used products.	(Linder et al., 2017)
Ease of Disassembly Metric (eDiM)	disassembly time of a product, based on time required for the different disassembly tasks for each component in the product.	(Vanegas et al., 2018)

Material criticality assessment

Innovators of materials and products should consider if their target materials or products are not dependent or vulnerable to supply of critical raw materials (CRMs). The EC evaluated and periodically updates a list of critical raw materials (CRMs) for the EU. The list of CRMs identified by the last assessment in 2023 includes 30 raw materials[8], some of them such as Li and Ni are also critical for energy storage devices. It should also be noted that recently, under the Green Deal, the EU has adopted the Critical Raw Material Act, which is specific regulation aiming to secure sustainable supply of critical raw materials for the development of critical industry sectors (European Parliament; Council of the European Union, 2024).

Criticality is based on supply risk of the material (entailing: possible export restrictions, that increase supply risk or possible trade agreements, that decrease it; the bottlenecks in the whole material's supply chain, not only the production stage; import dependency; and recycling, which may increase secondary supply and thus reduce supply risk), and economic importance (assessed by allocating raw material uses

[8] https://single-market-economy.ec.europa.eu/sectors/raw-materials/areas-specific-interest/critical-raw-materials_en

to their corresponding economic sectors; and by taking into account the possible substitution of the materials, which may reduce economic importance).

The critically assessment proposed here follows the EC SSbD guidance. Raw materials information is gathered along the innovation life cycle as part of the Safety and Environmental Assessment steps. This includes the specific materials in the innovation goal and materials that are used in the final product and applications. Materials are then checked if critical according to the EU CRM list.

5. Socio-economic assessment

Socio-economic assessment is an optional step in the SSbD framework. The step is not included in the EC Recommendation due to lower methodological maturity. Nevertheless, according to the new EU Battery Regulation, identifying social risks associated with a battery's supply chain becomes compulsory for battery manufacturers.

5.1. Sustainability: Social

Social sustainability assessment can be performed by means of Social LCA (S-LCA). The main methodological guidance is the UNEP Guidance (UNEP, 2020). The S-LCA methodology mirrors the Environmental LCA with four key phases: defining goals and scope, inventorying life cycle data, assessing impacts, and interpreting results.

Within the framework of SSbD, a simplified S-LCA can be employed to uncover potential social risks and opportunities within the supply chain of a chemical or material, and in the evaluation of alternatives.

The following steps are proposed:

1. Goal and scope definition:

- Identify organizations involved and their role in the different lifecycle stages of the product (e.g., supply chains). Where organizations are unknown, country-sector combinations of secondary data from S-LCA databases can be selected.
- Select which social topics (social endpoints) should be evaluated (e.g., local employment, child labor). This can be done through a materiality assessment, which is described in the European Sustainability Reporting Standard (ESRS).
- Define the stakeholder categories, i.e. groups of people affected (positively or negatively) by the product life cycle according to social topics selected.

2. Social inventory data

The assessment can be conducted with the help of databases such as the Product Social Impact Life Cycle Assessment database (PSILCA database)[9]. PSILCA was developed in compliance with the UNEP S-LCA guidelines and contains data for 19 subcategories and 65 qualitative and (semi-) quantitative indicators on social risks and impacts, covering around 15,000 country-specific industry sectors and commodities in 189 countries. The PSILCA database was used in LCA software such as OpenLCA.

S-LCA databases such as PSILCA have a low resolution (country/sector level for minerals), but this allows them to be comprehensive and cover a wide range of impacts. In this way, S-LCA can be used as an initial guide to identify potential hotspots along the supply chain.

3. Social impact assessment

The EC SSbD guideline suggests to assess the social performances and social risk along the whole life cycle according to the Reference Scale Approach (RSA). The approach is described in the guideline (Abbate et al., 2024) and exemplified in Caldeira et al. (2023).

[9] PSILCA—A Product Social Impact Life Cycle Assessment Database (GreenDelta). https://psilca.net/

As a further relevant example, Soeteman-Hernández et al. (2023) performed an S-LCA in their comparison of battery technologies, concluding that the majority of social impacts can be traced back to mining of metals and metalloids. Depending on the location and the type of mining that is required, different social risks may pose hotspots in the battery's supply chain.

5.2. Sustainability: Economic

The EC SSbD guideline proposes the Life Cycle Costing (LCC) methodology to assess economic considerations throughout the life cycle of the material/product subject to innovation. Environmental LCC (eLCC) is recommended, as it addresses both monetary costs and environmental externalities (Hoogmartens et al., 2014). Examples of studies that used LCC to compare batteries exist (e.g., (Baumann et al., 2017))

The Levelized Cost of Storage (LCOS) has been proposed by other researchers as indicator for economic sustainability (although purely financial) for energy storage technologies. LCOS is defined as ''the minimum price per kWh that a potential investor requires to break even over the entire lifetime of the storage facility'' (Comello and Reichelstein, 2019). A well-known and often cited analysis of LCOS of different types of batteries is published periodically by Lazard[10]. However, this indicator is usually calculated for more mature storage technologies rather than emerging designs that are still at pilot scale.

[10] https://www.lazard.com/media/42dnsswd/lazards-levelized-cost-of-storage-version-70-vf.pdf

6. Overall assessment of SSbD performance

The EC SSbD methodological guidance does not give much input to the process of overall assessment of SSbD performance. However, an approach is exemplified and tested with concrete cases studies in Caldeira et al. (2023). The scoring system proposed by Caldeira et al. (2023) is also adopted in the first version of the PARC toolbox (PARC, 2024). The approach is considered sufficient for the current framework.

The process of overall assessment can be understood as the approach to scoring innovations and references/ benchmarks in each SSbD step and the aggregation of these scores towards a total score. For the present framework this is illustrated in Figure 9.

As can be observed in Figure 9 aggregation of results is necessary at several hierarchical levels. Multi Criteria Decision Analysis (MCDA) methods can be used to perform this aggregation and several options exist (Cegan et al., 2017). The method selection should consider the goal of the SSbD assessment which may be different considering the innovation maturity level. Application of more complex MCDA methods, such as TOPSIS (Hwang and Yoon, 1981), have the potential to enhance SSbD scoring in the different steps.

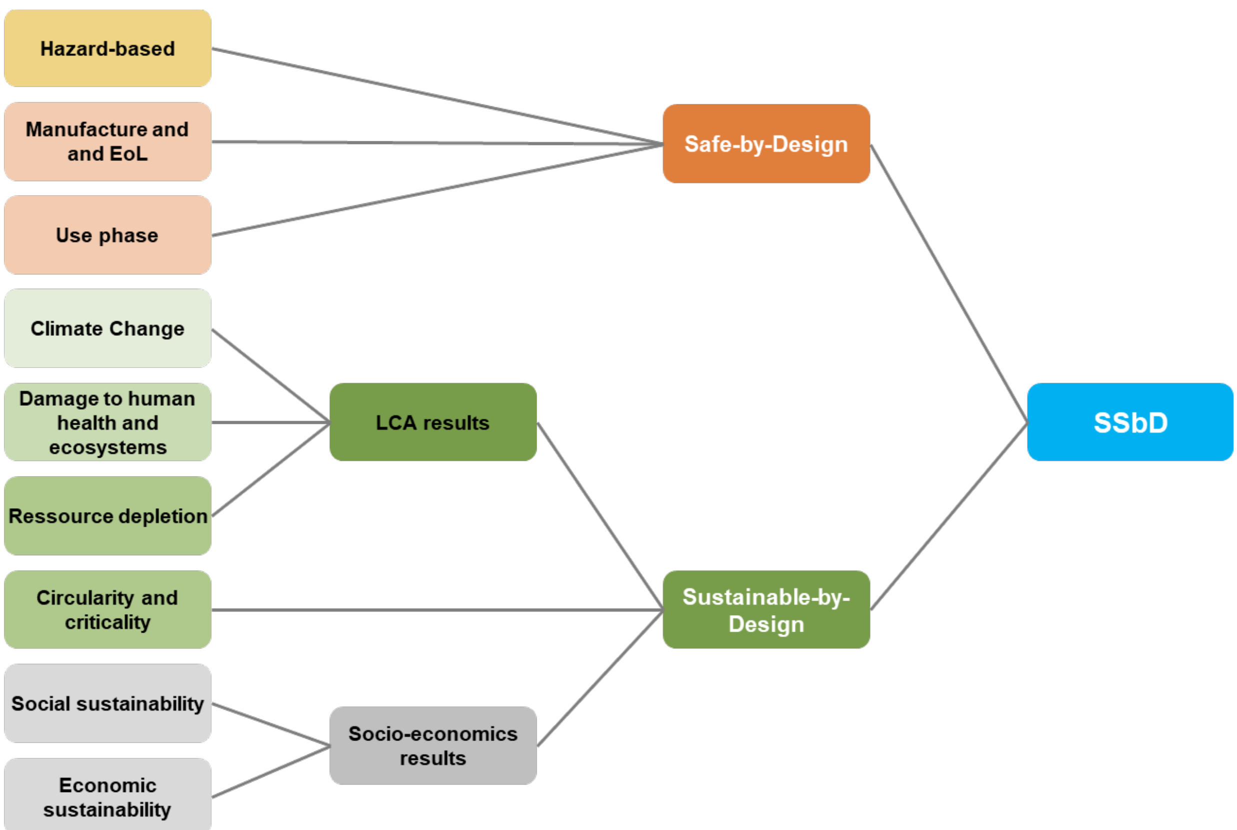

Figure 9: Hierarchical aggregation of SSbD results from different assessment steps.

7. Concluding remarks

SSbD is a framework recommended for guiding research and development, and for assessing and comparing innovation avenues. In this ARMS project deliverable, we outlined the framework customized for innovations addressing electrochemical energy storage devices.

The framework can be operationalized following the hierarchical approach described and considering the goal and level of innovation maturity. Safety aspects are evaluated first, followed by environmental (including circularity) aspects, social and economic aspects. The later may be considered optional but are generally important for innovations in electrochemical energy storage when certain materials are used.

The ARMS project develops new flexible and structural supercapacitors with high energy densities and based largely on environmentally friendly processes and materials. The project innovation maturity level starts at 3-4 with the goal of reaching 5-6 in the innovation areas addressed.

In the SSbD framework, the ARMS project falls within intermediate maturity range, necessitating a simplified SSbD approach to guide research and development processes. As summarized in Table 2, safety data sheets and predictive toolboxes like PARC are used to assess material and process safety for workers and consumers. Subsequently, LCA, simplified S-LCA, as well as LCC methods evaluate the sustainability of the developed supercapacitor from environmental, social and economic dimensions. The findings will identify critical materials and processes, pointing out the way for the development of a "green supercapacitor" with environmentally friendly applications.

8. Disclaimer

Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Commission. Neither the European Union nor the granting authority can be held responsible for them

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